

# OPTIMAL MULTISTEP METHODS FOR FIRST ORDER DIFFERENTIAL EQUATIONS IN HILBERT SPACES OF ANALYTIC FUNCTIONS

by

BRIJ BHUSHAN

MATH

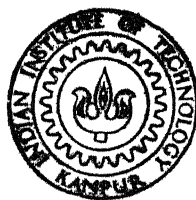
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DEPARTMENT OF MATHEMATICS  
INDIAN INSTITUTE OF TECHNOLOGY, KANPUR  
August., 1986

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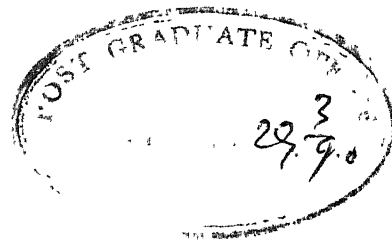
A Thesis Submitted  
in Partial Fulfilment of the Requirements  
for the Degree of  
**DOCTOR OF PHILOSOPHY**

by  
**BRIJ BHUSHAN**

to the  
DEPARTMENT OF MATHEMATICS  
INDIAN INSTITUTE OF TECHNOLOGY, KANPUR  
August., 1986



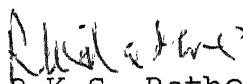
To  
My Parents



# CERTIFICATE

Certified that the work presented in this thesis entitled 'OPTIMAL MULTISTEP METHODS FOR FIRST ORDER DIFFERENTIAL EQUATIONS IN HILBERT SPACES OF ANALYTIC FUNCTIONS' by Mr. Brij Bhushan has been carried out under my supervision and that it has not been submitted elsewhere for a degree or diploma.

August - 1986

  
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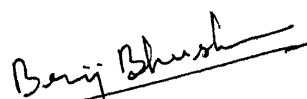
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August - 1986

  
(BRIJ BHUSHAN)

## SYNOPSIS

Sard's approach to optimal quadrature, resulting in a problem of linear best approximation, has been fruitfully investigated by many authors including Barnhill, Chawla, Davis, Kaul, Larkin, Rabinowitz, Richter, Raina, Valentin and others. In the area of multistep methods for ordinary differential equations, however, the basic potential of Sard's approach, to our best knowledge, has remained unexplored. The present thesis may, thus, be regarded as a first exploratory study of Sard's approach to optimal multistep methods.

Our adaptation of this approach to obtain 'optimal multistep formulae' may be summarized as follows. We begin with a basic multistep formula

$$Y_{n+1} = \sum_{i=1}^m a_i Y_{n+1-i} + h \sum_{j=0}^m b_j f(x_{n+1-j}, Y_{n+1-j}),$$

which, a priori, is known to be stable and convergent.

We retain the  $a_i$ 's of the formula as such and allow the  $b_j$ 's to be variables in writing down the norm of the local truncation error functional at the point  $x_{n+1}$ . Finally, the optimal  $b_j$ 's corresponding to the point  $x_{n+1}$  are obtained by minimizing this norm. (In principle one could have carried out the minimization also with respect to the  $a_i$ 's. However, this over-minimization, in general,

does not result in a stable multistep method even though the formulae thus obtained are locally highly accurate).

Keeping in mind that many of the classical multistep formulae adapt appropriate quadrature formulae to the differential equation situation, we have also considered multistep formulae based on optimal quadrature. Such formulae are distinct from the optimal multistep formulae and have been termed as 'quadrature optimal multistep formulae'.

Further, in addition to the purely optimal/quadrature optimal multistep formulae, the study also includes optimal/quadrature optimal formulae subject to certain interpolatory constraints.

The various formulae/methods of the thesis have been studied under: (a) derivation, (b) characterization, (c) numerical determination, (d) numerical application, (e) qualitative/quantitative properties and (f) convergence and error analysis.

A chapter-wise summary of the contents of the thesis is given below:

#### CONTENTS OF THE THESIS

The body of the thesis is divided into six chapters:

CHAPTER 1 is devoted to the derivation and characterization of quadrature optimal and optimal multistep formulae in the

general frame-work of a Hilbert space possessing a reproducing kernel function. The formulae with interpolatory constraints have been divided into two categories: one with interpolatory functions as polynomials of a certain degree and the other in which these functions are general, subject to their derivatives being linearly independent on the node sets of the formulae.

It is shown that at each step the coefficients of the formulae give rise to a deterministic system of linear equations and that each formula is characterized by its being interpolatory for a certain set of functions.

CHAPTERS 2-5 consist of a numerical implementation of the ideas of Chapter 1 to the case of two Hilbert spaces  $H^2(c_r)$  and  $L^2(\hat{c}_r)$  of analytic functions. Quadrature optimal multistep formulae/interpolatory for polynomials/general functions in the spaces  $H^2(\check{c}_r)$  and  $L^2(\hat{\check{c}}_r)$ , have been considered in Chapter 2 and Chapter 4, respectively; whereas, for the respective spaces, optimal multistep formulae/interpolatory for polynomials/general functions have been studied in Chapter 3 and Chapter 5. Each of these chapters contains: (1) the appropriate system of linear equations, particularly simplified for the space under consideration, for determination of multistep coefficients, (2) the functions for which the multistep formulae are characteristically interpolatory (3) numerical

tables of coefficients of optimal multistep formulae with Adams-Bashforth/Adams-Moulton as base formulae and (4) tabulated numerical results when these formulae are applied to a test set of twenty four differential equations. A numerical comparison of various multistep formulae occurring within each chapter has also been made.

In each of these chapters we have studied the limiting behaviour of the coefficients of optimal multistep formulae, as  $r \rightarrow \infty$ . It has been established that, in each case, the coefficients have limiting values equalling the coefficients of the corresponding usual formula which is of maximal polynomial precision with the same  $a_1$ 's and other interpolatory constraints.

The numerical results of Chapters 2-5 show that the various optimal multistep formulae for the spaces  $H^2(c_r)$  and  $L^2(\hat{c}_r)$  are quite accurate and superior to the corresponding usual formulae. The only disadvantage which the optimal formulae suffer from is that unlike in the classical multistep formulae the coefficients in these do not remain invariant over the steps.

CHAPTER 6 deals with a theoretical error analysis of various multistep formulae derived earlier. It is shown that the coefficients of the optimal multistep formulae in  $H^2(c_r)$  and  $L^2(\hat{c}_r)$  approach the coefficients of the corresponding usual formulae as the step size tends to zero.



In view of this fact, qualitative asymptotic stability properties of optimal multistep methods are to remain the same as those of the corresponding usual methods. However, since the coefficients of the optimal formulae vary from step to step, the various classical notions of stability and the associated stability regions, as such, fail to remain applicable to the optimal multistep methods. Consequently, for the optimal multistep methods a recourse is taken to the approach delineated by Henrici. We first show that the optimal methods are convergent. Next, a bound has been obtained on the accumulated discretization error in these methods. Finally, the propagation of round off errors in the application of the optimal methods has been studied.

## KEY TO SPECIAL SYMBOLS USED

$\int$	quadrature optimal case
$\wedge$	optimal case
$\cdot^P$	interpolatory for polynomials of a certain degree
$\cdot^F$	interpolatory for general functions
EUSUAL	norm of local truncation error functional for usual formula
EOPTIMAL	norm of local truncation error functional for optimal formula of a particular type
EEO	<u>e</u> rror in <u>e</u> xplicit <u>o</u> ptimal type case
EEU	<u>e</u> rror in <u>e</u> xplicit <u>u</u> sual case
EIO	<u>e</u> rror in <u>i</u> mplicit <u>o</u> ptimal type case
EIU	<u>e</u> rror in <u>i</u> mplicit <u>u</u> sual case
ITO	number of <u>i</u> terations in <u>o</u> ptimal type case
ITU	number of <u>i</u> terations in <u>u</u> sual case
$H \times B(i)$	numerical coefficient of $f(x_{n+1-i}, y_{n+1-i})$ in a formula

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## CHAPTER 1

### OPTIMAL AND QUADRATURE OPTIMAL MULTISTEP METHODS AND THEIR CHARACTERIZATIONS

#### 1.1 Introduction

Many of the classical multistep methods are based on quadrature formulae with polynomial precision. For an initial value problem (IVP)

$$(1) \quad \begin{aligned} y' &= f(x, y) \\ y(x_0) &= y_0 \end{aligned}$$

one considers

$$Y_{n+1} - Y_{n-s} = \int_{x_{n-s}}^{x_{n+1}} f(x, y) dx$$

and approximates the integral occurring on the right hand side by a discrete quadrature formula of the type

$$\int_{x_{n-s}}^{x_{n+1}} f(x, y) dx = h \sum b_j f(x_{n+1-j}, Y_{n+1-j}),$$

$j$  varying over an appropriate set. The coefficients  $b_j$ 's are chosen according to some appropriate criteria. The choice of the coefficients  $b_j$ 's in the classical quadrature based Adams-Bashforth/Adams-Moulton, Nystrom/Milne-Simpson formulae (Henrici [27], Jain [28], Lapidus [31]) is so as to make the formula locally exact for polynomials of a degree as large as possible.

A more generalized approach is to consider a multistep method of the type

$$Y_{n+1} = \sum a_i Y_{n+1-i} + h \sum b_j f(x_{n+1-j}, Y_{n+1-j})$$

where the coefficients  $a_i$ 's and  $b_j$ 's are chosen so as to have a balance of precision and stability properties in the method (Henrici [27], Jain [28]). The precision with respect to the polynomial functions renders the coefficients  $a_i$ 's and  $b_j$ 's independent of  $x_n$ . This property of coefficients is retained even when the formulae are made interpolatory for the exponential functions  $e^{ax}$ . However if the formulae are made interpolatory with respect to a general class of functions the coefficients  $a_i$ 's and  $b_j$ 's would no more be independent of the point  $x_n$  under consideration.

Beginning with the work of Sard in 1949, much work has been done on quadrature rules of minimum error norm corresponding to various classes of functions. Sard [42], Davis [19], Valentin [44], Barnhill [3], [4], [5], [6], [8], [9], Barnhill and Wixom [10], Barrar [13] and Larkin [32] have considered minimization of quadrature error in different manners with respect to weights (and nodes) to get optimal rules. Pinkus [34], Rabinowitz and Richter [35], [36], Richter [39], [40], [41] have studied properties of such rules. Chawla and Kaul [16], [17], [18] and Kaul [30] considered such optimal rules subject to interpolatory conditions for polynomials of

of degree less than or equal to the number of nodes. Kaul [30] and Finney and Price Jr. [24] have studied optimal rules with interpolating conditions for arbitrary functions.

No similar approach to get optimal formulae in numerical solution of differential equations, however, seems to have been taken up in the literature even though a need for this has been felt for quite some time (Gear [25]).

The present thesis is an approach in this direction and consists of a study of such methods which minimize the quadrature error or local truncation error in the numerical integration of a first order initial value problem.

This chapter is devoted to the derivation of the various formulae and their characterization. Implementation of these formulae is done in next four chapters for two Hilbert spaces of practical interest. The last chapter of the thesis is a study of the error analysis of these methods.

We develop multistep methods for the initial value problem (1) by minimizing the norm of local truncation error of multistep methods in various fashions over a Hilbert space of analytic functions possessing a reproducing kernel function.

A Hilbert space  $H$  of functions  $y(x)$  on a domain  $B$  possesses a reproducing kernel function  $K(x, \bar{t})$  if, and



only if, for every  $x \in B$  the linear functional  $I_x(y) = y(x)$  is bounded over  $H$ . This is the well known result of Aronszajn (Davis [22], Theorem 12.6.1). The reproducing kernel function  $K(x, \bar{t})$  possesses the following property. For each fixed  $t \in B$ ,  $K(x, \bar{t}) \in H$  and

$$y(t) = (y(x), K(x, \bar{t}))$$

for every  $y \in H$  where  $(\dots)$  denotes the inner product in  $H$ . It then follows that the kernel function is unique and for  $x, t \in B$

$$K(t, \bar{x}) = \overline{K(x, \bar{t})}$$

In this chapter we assume that the  $k$ th derivative evaluation functional  $D_x^k: f \mapsto f^{(k)}(x)$  is, for  $k=1$ , a bounded linear functional in  $H$  for every  $x \in B$ . Further, we shall assume that  $H$  contains, as a subspace, the set of all polynomial functions.

In Section 1.2 of this chapter we obtain and characterize multistep methods which are obtained by minimizing the quadrature error over a Hilbert space. In Section 1.3 the formulae are subjected to precision for polynomials of certain degree along with the minimization of quadrature error. In Section 1.4 interpolatory conditions are developed for a general set of preassigned functions subject to which the quadrature error is minimized over the Hilbert space. The rest of the chapter follows the spirit of a general multistep method

where the norm of local truncation error rather than the local quadrature error is subjected to minimization. Thus in Section 1.5 we obtain the coefficients of multistep method by minimizing the norm of local truncation error over the space. In Section 1.6 the truncation error is minimized subject to polynomial precision, while in Section 1.7 the same has been done with precision for an arbitrary set of preassigned functions. In all these cases the formulae obtained have been shown to get characterized by interpolatory conditions for a certain set of functions.

## 1.2 Quadrature Optimal Multistep Methods ( $\tilde{M}$ )

A multistep method

$$(2) \quad Y_{n+1} - Y_{n-s} = h \sum_{i=\delta_{t0}}^m \tilde{b}_i f(x_{n+1-i}, Y_{n+1-i}), \quad 0 \leq s < m,$$

where  $\delta_{ij}$  is the Kronecker delta, for the initial value problem (1) represents an explicit method if  $t=0$  and implicit method if  $t=1$ . Local truncation error  $\tilde{T}_n$  for the method is given by

$$\begin{aligned} \tilde{T}_n y &= y(x_{n+1}) - Y_{n+1} \\ &= y(x_{n+1}) - Y_{n-s} - h \sum_{i=\delta_{t0}}^m \tilde{b}_i y'_{n+1-i} \end{aligned}$$

Regarding (2) as a quadrature based multistep method the coefficients  $\tilde{b}_i$ 's are ones corresponding to the quadrature rule

$$\int_{x_{n-s}}^{x_{n+1}} F(x) dx \approx h \sum_{i=\delta_{t_0}}^m \tilde{b}_i F(x_{n+1-i})$$

The quadrature error is given by

$$Q_n(F) = \int_{x_{n-s}}^{x_{n+1}} F(x) dx - h \sum_{i=\delta_{t_0}}^m \tilde{b}_i F(x_{n+1-i})$$

and the representer of this quadrature error functional  $Q_n$  is given by

$$(3) \quad Q_n = g_n(t) - h \sum_{i=\delta_{t_0}}^m \tilde{b}_i K(t, \bar{x}_{n+1-i})$$

where  $g_n(t)$  denotes the representer of the linear functional corresponding to the integral evaluation:  $F \rightarrow \int_{x_{n-s}}^{x_{n+1}} F(x) dx$  and

$K(x, \bar{t})$  is the kernel function of the Hilbert space. To determine the coefficients of a quadrature optimal method (2) we minimize  $\|Q_n\|^2$  with respect to  $\tilde{b}_i$ 's, where

$$(4) \quad \|Q_n\|^2 = (g(t) - h \sum_{i=\delta_{t_0}}^m \tilde{b}_i K(t, \bar{x}_{n+1-i}), \\ g(t) - h \sum_{j=\delta_{t_0}}^m \tilde{b}_j K(t, x_{n+1-j}))$$

Following Larkin [32] the first order change  $\delta(\|Q_n\|^2)$  in  $\|Q_n\|^2$ , following a change  $\delta(\tilde{b}_k)$  in  $\tilde{b}_k$ , is given by

$$\begin{aligned}
\delta(\|Q_n\|^2) &= -h(\delta(\tilde{b}_k)K(t, \bar{x}_{n+1-k}), g(t) - h \sum_{j=\delta_{to}}^m \tilde{b}_j K(t, \bar{x}_{n+1-j})) \\
&\quad - h(g(t) - h \sum_{i=\delta_{to}}^m \tilde{b}_i K(t, \bar{x}_{n+1-i}), \delta(\tilde{b}_k)K(t, \bar{x}_{n+1-k})) \\
(5) \quad &= -h \overline{\delta(\tilde{b}_k) (g(x_{n+1-k}) - h \sum_{j=\delta_{to}}^m \tilde{b}_j K(x_{n+1-k}, \bar{x}_{n+1-j}))} \\
&\quad - h \delta(\tilde{b}_k) (g(x_{n+1-k}) - h \sum_{i=\delta_{to}}^m \tilde{b}_i K(x_{n+1-k}, \bar{x}_{n+1-i}))
\end{aligned}$$

Since, for minimizing  $\tilde{b}_k$ 's,  $\delta(\|Q_n\|^2)$  has to vanish for an arbitrary choice of  $\delta(\tilde{b}_k)$ , we have

$$(6) \quad h \sum_{j=\delta_{to}}^m K(x_{n+1-j}, \bar{x}_{n+1-k}) \tilde{b}_j = \overline{g(x_{n+1-k})}, \quad k = \delta_{to}(1)m$$

The matrix  $[K(x_{n+1-j}, \bar{x}_{n+1-k})]_{k,j=\delta_{to}}^m$  of the linear system,

being a Gram matrix for distinct  $x_{n+1-j}$ ,  $j = \delta_{to}(1)m$ , is non-singular (Davis [22]). Hence the system of linear equations given by (6) has unique solution.

Note that we have minimized only the quadrature error. The norm of local truncation error  $\tilde{T}_n$  is given by

$$(7) \quad \|\tilde{T}_n\| = \|K(t, \bar{x}_{n+1}) - K(t, \bar{x}_{n-s}) - h \sum_{i=\delta_{to}}^m \tilde{b}_i D(t, \bar{x}_{n+1-i})\|$$

where  $D(t, \bar{x}_{n+1-i})$  is the representer of the derivative functional evaluation at the point  $\bar{x}_{n+1-i}$ . For the purpose of evaluation of the norm of local truncation error it is assumed that derivative is a bounded linear functional.

Now we prove:

Theorem 1. The quadrature optimal multistep method  $(\tilde{M})$  given by (2) is characterized by that it is locally interpolatory for functions  $\{h_j(x), j = \delta_{t_0}(1)m\}$  with

$$h_j(x) = \int^x K(x, \bar{x}_{n+1-j}) dx,$$

$\int^x$  standing for an indefinite integral operation.

Proof: From (6) we observe that the multistep method (2) is exactly satisfied by the functions whose derivatives are

$$K(x, \bar{x}_{n+1-k}), \quad k = \delta_{t_0}(1)m$$

Hence the result.

### 1.3 Quadrature Optimal Multistep Methods Interpolatory for Polynomials $(\tilde{M}^p)$

A quadrature multistep formula

$$(8) \quad y_{n+1} - y_{n-s} = h \sum_{i=\delta_{t_0}}^m \tilde{b}_i^p f(x_{n+1-i}, y_{n+1-i})$$

is interpolatory for polynomials upto degree  $p$  if it is satisfied exactly by polynomials of degree  $p$ , that is by any linearly independent polynomials  $q_1 \dots q_p$  in the span  $\{x^i; 1 \leq i \leq p\}$ . Since the method is obviously exact for constants we donot include constants in this set. Let

$$(9) \quad l_{pj}(x) = \prod_{\substack{k=\delta_{t_0} \\ k \neq j}}^{p-1+\delta_{t_0}} \left( \frac{x - x_{n+1-k}}{x_{n+1-j} - x_{n+1-k}} \right), \quad j = \delta_{t_0}(1)p - 1 + \delta_{t_0}$$

and let

$$(10) \quad q_{pj}(x) = \int_0^x l_{pj}(x) dx, \quad j = \delta_{t_0}(1)p-1+\delta_{t_0}.$$

Because  $l_{pj}(x)$  are linearly independent and form a basis for  $\text{span}\{1, x, \dots, x^{p-1}\}$ ,  $q_{pj}(x)$  are linearly independent and form a basis for  $\text{span}\{x, x^2, \dots, x^p\}$ . Therefore we get

$$q_{pj}(x_{n+1}) - q_{pj}(x_{n-s}) = h b_j^p + h \sum_{k=p+\delta_{t_0}}^m \tilde{b}_k^p l_{pj}(x_{n+1-k}).$$

Thus

$$(11) \quad \tilde{h} b_j^p = q_{pj}(x_{n+1}) - q_{pj}(x_{n-s}) - \sum_{k=p+\delta_{t_0}}^m h \tilde{b}_k^p l_{pj}(x_{n+1-k}),$$

$$j = \delta_{t_0}(1)p-1+\delta_{t_0}.$$

The norm of quadrature error is thus given by

$$(12) \quad |||Q_n^p||| = |||g_n(t) - h \sum_{k=\delta_{t_0}}^m \tilde{b}_k^p K(t, \bar{x}_{n+1-k})|||$$

$$= |||g_n(t) - \sum_{j=\delta_{t_0}}^{p-1+\delta_{t_0}} \frac{q_{pj}(x_{n+1}) - q_{pj}(x_{n-s})}{\{q_{pj}(x_{n+1}) - q_{pj}(x_{n-s})\}} K(t, \bar{x}_{n+1-j})$$

$$- h \sum_{k=p+\delta_{t_0}}^m \tilde{b}_k^p \{K(t, \bar{x}_{n+1-k}) - \sum_{j=\delta_{t_0}}^{p-1+\delta_{t_0}} l_{pj}(x_{n+1-k})$$

$$K(t, \bar{x}_{n+1-j})\}|||.$$

Let

$$(13) \quad s_{np}(t; \bar{x}_{n+1-k}) = K(t, \bar{x}_{n+1-k}) - \sum_{j=\delta_{t_0}}^{p-1+\delta_{t_0}} \frac{l_{pj}(x_{n+1-k})}{\{q_{pj}(x_{n+1}) - q_{pj}(x_{n-s})\}} K(t, \bar{x}_{n+1-j})$$

and

$$(14) \quad r_{np}(t) = g_n(t) - \sum_{j=\delta_{t_0}}^{p-1+\delta_{t_0}} \frac{\{q_{pj}(x_{n+1}) - q_{pj}(x_{n-s})\} K(t, \bar{x}_{n+1-j})}{\delta_{t_0}}.$$

Then

$$(15) \quad \|Q_n^p\| = \|r_{np}(t) - h \sum_{k=p+\delta_{t_0}}^m \tilde{b}_k^p s_{np}(t; \bar{x}_{n+1-k})\|.$$

The functions  $s_{np}(t, \bar{x}_{n+1-k})$ ,  $k=p+\delta_{t_0}(1)m$  are linearly independent (Lemma 1.1 Kaul [30]), for distinct points  $x_{n+1-k}$ ,  $k=\delta_{t_0}(1)m$ . Therefore minimizing  $\|Q_n^p\|$  with respect to  $\tilde{b}_k^p$  is equivalent to finding the best least square approximation to  $r_n(t)$  by a linear combination of the linearly independent functions  $\{s_{np}(t; \bar{x}_{n+1-k}) ; k = p+\delta_{t_0}(1)m\}$ ; therefore the coefficients  $\tilde{b}_k^p$ ,  $k=p+\delta_{t_0}(1)m$  giving the best approximation are obtained by solving (Davis [22], Theorem (8.6.3)) the system of linear equations.

$$(16) \quad (r_{np}(t) - \sum_{k=p+\delta_{t_0}}^m \tilde{b}_k^p s_{np}(t; \bar{x}_{n+1-k}), s_{np}(t; \bar{x}_{n+1-j})) = 0, \\ j = p + \delta_{t_0}(1)m.$$

That is

$$(17) \quad \sum_{k=p+\delta_{t_0}}^m a_{jk} \tilde{b}_k^p = d_j,$$

where we have set

$$(18) \quad a_{jk} = (s_{np}(t; \bar{x}_{n+1-j}), s_{np}(t; \bar{x}_{n+1-k}))$$

and

$$(19) \quad d_j = (s_{np}(t; \bar{x}_{n+1-j}), r_{np}(t)).$$

From (18) and (19) we get

$$(20) \quad a_{jk} = s_{np}(x_{n+1-k}; \bar{x}_{n+1-j}) - \sum_{i=p+\delta_{t_0}}^{p-1+\delta_{t_0}} l_{pi}(x_{n+1-k}) s_{np}(x_{n+1-i}; \bar{x}_{n+1-j})$$

and

$$(21) \quad \bar{d}_j = r_{np}(x_{n+1-j}) - \sum_{i=p+\delta_{t_0}}^{p-1+\delta_{t_0}} l_{pi}(x_{n+1-j}) r_{np}(x_{n+1-i}),$$

$$j, k = p+\delta_{t_0}(1)m.$$

The matrix  $[a_{jk}]_{j,k=p+\delta_{t_0}}^m$  is Gram matrix for linearly independent functions  $\{s_{np}(t; \bar{x}_k); k=p+\delta_{t_0}(1)m\}$  and hence it is non-singular. The  $\tilde{b}_j^p$  are unique at all points  $x_{n+1}$ .

Theorem 2: The quadrature optimal multistep method interpolatory for polynomials of degree  $p < m+\delta_{t_1}$  is characterized by that it is locally interpolatory for functions

$$\{x^i; 0 \leq i \leq p\} \cup \{h_j; j = p+\delta_{t_0}(1)m\}$$

where

$$h_j(x) = \int_x^x s_{np}(x; \bar{x}_{n+1-j}) dx.$$

Proof: Obviously the method (8) is exact for constants and  $\{x^i; 1 \leq i \leq p\}$ . From (16) it follows that the method is exact for indefinite integral of  $s_{np}(x; \bar{x}_{n+1-j})$ , the method being quadrature based. Hence the result.



#### 1.4 Quadrature Optimal Multistep Methods Interpolatory for Arbitrary Functions ( $\tilde{M}^F$ )

A quadrature multistep method

$$(22) \quad Y_{n+1} - Y_{n-s} = h \sum_{j=\delta_{to}}^m \tilde{b}_j^F f(x_{n+1-j}, Y_{n+1-j})$$

is called interpolatory for linearly independent functions  $\{\varphi_1, \dots, \varphi_p\}$  if it is exact for these functions and if also the quadrature error is minimal, it is called optimal interpolatory.

We assume that the matrix  $[\varphi'_i(x_{n+1-j})]_{i=1, j=\delta_{to}}^{p, p-1+\delta_{to}}$  is non-singular where  $\varphi'_i(x_{n+1-j})$  denotes the derivative of  $\varphi_i$  at point  $x_{n+1-j}$ . Differentiability of functions  $\{\varphi_1, \dots, \varphi_p\}$  is a must, otherwise they cannot satisfy a differential equations. Let

$$(23) \quad f_{pi}(x) = \sum_{j=\delta_{to}}^{p-1+\delta_{to}} c_{ij} \varphi_{j+1-\delta_{to}}(x), \quad i=1, \dots, p$$

where  $[c_{ij}] = [\varphi'_i(x_{n+1-j})]^{-1}$ . Obviously  $\{f_{p1}, \dots, f_{pp}\}$  are linearly independent and

$$(24) \quad \begin{aligned} f'_{pi}(x_{n+1-k}) &= \sum_{j=\delta_{to}}^{p-1+\delta_{to}} c_{ij} \varphi'_{j+1-\delta_{to}}(x_{n+1-k}) \\ &= \delta_{ik+1-\delta_{to}} \end{aligned}$$

The functions  $\{f_{p1}, \dots, f_{pp}\}$  form a basis for  $\text{span}\{\varphi_1, \dots, \varphi_p\}$ , and thus if the method (22) is interpolatory for functions

$\{f_{p1}, \dots, f_{pp}\}$  it will be interpolatory for functions  $\{\varphi_1, \dots, \varphi_p\}$ .

Substituting  $f_{pi}$  in (22) we get

$$f_{pi}(x_{n+1}) - f_{pi}(x_{n-s}) = h \tilde{b}_{i-1+\delta_{to}}^F + h \sum_{j=p+\delta_{to}}^m \tilde{b}_j^F f'_{pi}(x_{n+1-j})$$

giving

$$(25) \quad h \tilde{b}_{i-1+\delta_{to}}^F = f_{pi}(x_{n+1}) - f_{pi}(x_{n-s}) - h \sum_{j=p+\delta_{to}}^m \tilde{b}_j^F f'_{pi}(x_{n+1-j}),$$

$i=1(1)p.$

Let  $Q_n^F$  denote the quadrature error in method (22). Then, proceeding similarly as in Section 1.3 we have

$$(26) \quad \begin{aligned} ||Q_n^F|| &= ||g_n(t) - h \sum_{k=\delta_{to}}^m \tilde{b}_k^F K(t, x_{n+1-k})|| \\ &= ||r_{np}^F(t) - h \sum_{k=p+\delta_{to}}^m \tilde{b}_k^F s_{np}^F(t, \bar{x}_{n+1-k})|| \end{aligned}$$

where

$$(27) \quad s_{np}^F(t; \bar{x}_{n+1-k}) = K(t, \bar{x}_{n+1-k}) - \sum_{j=\delta_{to}}^{p-1+\delta_{to}} \frac{f'_{p,j+1-\delta_{to}}(x_{n+1-k})}{K(t, \bar{x}_{n+1-j})}.$$

$$(28) \quad r_{np}^F(t) = g_n(t) - \sum_{j=\delta_{to}}^{p-1+\delta_{to}} \frac{\{f_{pj+1-\delta_{to}}(x_{n+1}) - f_{pj-\delta_{to}}(x_{n-s})\}}{K(t, \bar{x}_{n+1-j})}.$$

Lemma 1: The functions  $s_{np}^F(t; \bar{x}_{n+1-k})$ ,  $k=p+\delta_{to}(1)m$  are linearly independent in  $H$ .

Proof: Let

$$\sum_{k=p+\delta_{to}}^m \alpha_k s_{np}^F(t; \bar{x}_{n+1-k}) = 0.$$

Then we define  $f_{mi}(x)$  for a linearly independent set  $\{\varphi_1, \dots, \varphi_m\}$  of differentiable functions as in (23). Then

$$\begin{aligned} 0 &= (f'_{mi}(t), 0) \\ (29) \quad &= (f'_{mi}(t), \sum_{k=p+\delta_{to}}^m \alpha_k s_{np}^F(t; \bar{x}_{n+1-k})) \\ &= \sum_{k=p+\delta_{to}}^m \bar{\alpha}_k (f'_{mi}(t), s_{np}^F(t; \bar{x}_{n+1-k})). \end{aligned}$$

Now, with  $[\varphi'_i(x_{n+1-j})]_{i,j=1}^m$  non-singular so that  $f'_{mi}(x_{n+1-j}) = \delta_{ij}$ ,

$$\begin{aligned} &-(f'_{mi}(t), s_{np}^F(t; \bar{x}_{n+1-k})) \\ &= f'_{mi}(x_{n+1-k}) - \sum_{j=\delta_{to}}^{p-1+\delta_{to}} f'_{pj+1-\delta_{to}}(x_{n+1-k}) f'_{mi}(x_{n+1-j}) \\ &= \delta_{ik} - \sum_{j=\delta_{to}}^{p-1+\delta_{to}} f'_{pj+1-\delta_{to}}(x_{n+1-k}) \delta_{ij} \\ &= \delta_{ik}, \quad i, k = p+\delta_{to}(1)m. \end{aligned}$$

Substituting in (29) we get  $\alpha_k = 0, k = p+\delta_{to}(1)m$ , which proves the lemma.

Hence the coefficients  $\tilde{b}_{k,k=p+\delta_{to}(1)m}^F$  which minimize  $\|Q_n^F\|$  given by (26) can be determined by solving a system of linear equations

$$(30) \quad \sum_{k=p+\delta_{t_0}}^m a_{jk}^F \tilde{b}_k^F = d_j^F$$

where we have set

$$a_{jk}^F = (s_{np}^F(t; \bar{x}_{n+1-j}), s_{np}^F(t; \bar{x}_{n+1-k})),$$

and

$$d_j = (s_{np}^F(t; \bar{x}_{n+1-j}), r_{np}^F(t)), \quad j, k = p + \delta_{t_0}(1)m$$

From these and using the properties of the kernel function we can easily obtain

$$\begin{aligned} a_{jk}^F &= s_{np}^F(x_{n+1-k}, \bar{x}_{n+1-j}) - \sum_{i=\delta_{t_0}}^{p-1+\delta_{t_0}} f_{pi+1-\delta_{t_0}}^F(x_{n+1-k}) \cdot \\ &\quad \cdot s_{np}^F(x_{n+1-i}, \bar{x}_{n+1-j}) \\ \bar{d}_j &= r_{np}^F(x_{n+1-j}) - \sum_{i=\delta_{t_0}}^{p-1+\delta_{t_0}} f_{pi+1-\delta_{t_0}}^F(x_{n+1-j}) r_{np}^F(x_{n+1-i}), \\ &\quad j, k = p + \delta_{t_0}(1)m. \end{aligned}$$

The matrix  $[a_{jk}^F]_{j,k=p+\delta_{t_0}}^m$  is gram matrix for linearly independent functions  $s_{np}^F(t; \bar{x}_{n+1-k})$ ,  $k=p+\delta_{t_0}(1)m$ , and hence it is non-singular. Thus  $\tilde{b}_j^F$  can be determined uniquely from (25) and (30). Now we can prove :

Theorem 3: The quadrature optimal multistep method (22), interpolating the functions  $\{\varphi_1, \varphi_2, \dots, \varphi_p\}$ , is characterized by that it is interpolatory for constants and

$$\{f_{pi} : i=1(1)p\} \cup \{h_j^F : j = p + \delta_{t_0}(1)m\}$$

where

$$h_j^F(x) = \int^x s_{np}^F(x, \bar{x}_{n+1-j}) dx.$$

Proof: The proof is similar to that of Theorem 2.

### 1.5 Optimal Multistep Methods (M)

In this and the subsequent sections we develop the methods which minimize local truncation error instead of the quadrature error. Since the stability properties of a multistep method depend strongly on the choice of  $a_i$ 's our major emphasis is on the development of optimal methods of the form

$$(31) \quad Y_{n+1} = \sum_{i=1}^m a_i Y_{n+1-i} + h \sum_{j=\delta_{to}}^m \hat{b}_j f(x'_{n+1-j}, Y_{n+1-j}),$$

where  $a_i$ 's are prefixed according to a known stable classical multistep method, the optimality criterion being the minimization of the norm of local truncation error functional.

The local truncation error functional  $\hat{T}_n$  of an optimal multistep method applied to a function  $y(x)$  is given by

$$(32) \quad \begin{aligned} \hat{T}_n y &= y(x_{n+1}) - Y_{n+1} \\ &= Y_{n+1} - \sum_{i=1}^m a_i Y_{n+1-i} - h \sum_{j=\delta_{to}}^m \hat{b}_j y'_{n+1-j}. \end{aligned}$$

Therefore

$$(33) \quad ||\hat{T}_n|| = ||K(t, \bar{x}_{n+1}) - \sum_{i=1}^m \bar{a}_i K(t, \bar{x}_{n+1-i}) - h \sum_{j=\delta_{to}}^m \bar{b}_j D(t, \bar{x}_{n+1-j})||$$

where  $D(t, \bar{x}_{n+1-j})$  designates the representer of derivative evaluation at  $x_{n+1-j}$ . It has been assumed that the derivative evaluation is a bounded functional in  $H$ , with

$$(34) \quad D(t, \bar{x}_{n+1-j}) = \overline{\frac{\partial}{\partial x} K(x, \bar{t})} \Big|_{x=x_{n+1-j}}.$$

For determining  $\hat{b}_j, j=\delta_{to}(1)m$  such that the norm of the local truncation error is minimal in the method (31), we minimize  $||\hat{T}_n||$  with respect to  $\hat{b}_j$ 's. We establish:

Lemma 2: Let  $S = \{K(t, \bar{x}_{n+1-i}), D(t, \bar{x}_{n+1-i}) : i = o(1)m\}$ , for distinct points  $x_{n+1}, x_n, \dots, x_{n+1-m}$ . Then  $S$  is a linearly independent set.

Proof: We know that if  $x_{n+1-i}, i=o(1)m$  are  $m+1$  distinct points the basic Hermite interpolation polynomials  $P_{2m+1,k}$   $Q_{2m+1,k}$  satisfying

$$(35) \quad \begin{aligned} P_{2m+1,k}(x_{n+1-i}) &= \delta_{ik} , \\ Q_{2m+1,k}(x_{n+1-i}) &= 0 , \\ P'_{2m+1,k}(x_{n+1-i}) &= 0 , \\ Q'_{2m+1,k}(x_{n+1-i}) &= \delta_{ik} , \quad k = o(1)m , \end{aligned}$$

form a basis for polynomials upto degree  $2(m+1)-1$  (Ralston and Rabinowitz [38], p. 70). Let

$$(36) \quad \sum_{i=0}^m c_i K(t, \bar{x}_{n+1-i}) + \sum_{j=0}^m d_j D(t, \bar{x}_{n+1-j}) \equiv 0.$$

Then taking the inner product of (36) with functions  $P_{2m+1,k}(t)$ ,  $Q_{2m+1,k}(t)$ ,  $k = o(1)m$  we get

$$c_k = 0, \quad d_k = 0, \quad k = o(1)m,$$

Completing the proof.

Since  $S$  is linearly independent, to determine the optimal coefficients  $\hat{b}_j$ ,  $j = \delta_{t_0}(1)m$ , which minimize the norm of local truncation error  $\|\hat{T}_n\|$ , proceeding as in Section 1.2, we have

$$\begin{aligned} h \sum_{j=\delta_{t_0}}^m (D(t, \bar{x}_{n+1-k}), D(t, \bar{x}_{n+1-j})) \hat{b}_j \\ = (D(t, \bar{x}_{n+1-k}), K(t, x_{n+1}) - \sum_{i=1}^m \bar{a}_i K(t, x_{n+1-i})) , \\ k = \delta_{t_0}(1)m. \end{aligned}$$

Since

$$\begin{aligned} (D(t, \bar{x}_{n+1-k}), D(t, \bar{x}_{n+1-j})) \\ = \frac{\partial}{\partial t} D(t, \bar{x}_{n+1-k}) \Big|_{t=x_{n+1-j}} \\ = D'(x_{n+1-j}, \bar{x}_{n+1-k}), \quad (\text{say}) \end{aligned}$$

we have

$$\begin{aligned}
 (37) \quad h \sum_{j=\delta_{t_0}}^m D'(x_{n+1-j}, \bar{x}_{n+1-k}) \hat{b}_j \\
 = D(x_{n+1}, \bar{x}_{n+1-k}) - \sum_{i=1}^m a_i D(x_{n+1-i}, \bar{x}_{n+1-k}), \\
 k = \delta_{t_0}(1)m.
 \end{aligned}$$

From equations (37) we get following theorem:

Theorem 4: The optimal multistep method (31) where  $a_i$ ,  $i = 1(1)m$  are prefixed is characterized by that it is locally interpolatory for functions

$$\{D(x, \bar{x}_{n+1-j}), j = \delta_{t_0}(1)m\}.$$

Lemma 2 indicates that if the minimization of the local truncation error is done also with respect to  $a_i$ 's, the system of linear equations thus obtained will have a non-singular matrix and that such a formula will also be unique. However such formulae may not possess the stability properties required in a multistep method for the whole interval. Such a formula may be useful where the major interest is the minimization of the local truncation error (e.g. in the beginning of interval or at the point where the solution may be fast changing), nevertheless.

If the minimization in (33) is done with respect to both  $a_i$ 's and  $\hat{b}_j$ 's, the normal equations are



$$\begin{aligned}
& \sum_{k=1}^m (K(t, \bar{x}_{n+1-i}), K(t, \bar{x}_{n+1-k})) a_k \\
& + h \sum_{l=\delta_{t_0}}^m (K(t, \bar{x}_{n+1-i}), D(t, \bar{x}_{n+1-l})) \hat{b}_l \\
& = (K(t, \bar{x}_{n+1-i}), K(t, \bar{x}_{n+1})) , i=1(1)m
\end{aligned}$$

and

$$\begin{aligned}
& \sum_{k=1}^m (D(t, \bar{x}_{n+1-j}), K(t, \bar{x}_{n+1-k})) a_k \\
& + h \sum_{l=\delta_{t_0}}^m (D(t, \bar{x}_{n+1-j}), D(t, \bar{x}_{n+1-l})) \hat{b}_l \\
& = (D(t, \bar{x}_{n+1-j}), K(t, \bar{x}_{n+1})) , j = \delta_{t_0}(1)m
\end{aligned}$$

which simplify to

$$\begin{aligned}
& \sum_{k=1}^m K(x_{n+1-k}, \bar{x}_{n+1-i}) a_k + h \sum_{l=\delta_{t_0}}^m K'(x_{n+1-l}, \bar{x}_{n+1-i}) \hat{b}_l \\
(38) \quad & = K(x_{n+1}, \bar{x}_{n+1-i}) , i=1(1)m , \text{ and}
\end{aligned}$$

$$\begin{aligned}
& \sum_{k=1}^m D(x_{n+1-k}, \bar{x}_{n+1-j}) a_k + h \sum_{l=\delta_{t_0}}^m D'(x_{n+1-l}, \bar{x}_{n+1-j}) \hat{b}_l \\
& = D(x_{n+1}, \bar{x}_{n+1-j}) , j = \delta_{t_0}(1)m.
\end{aligned}$$

From these  $2m + \delta_{t_0}$  equations we conclude:

Theorem 5: An optimal multistep method given by

$$(39) \quad y_{n+1} = \sum_{i=1}^m \hat{a}_i y_{n+1-i} + h \sum_{j=\delta_{t_0}}^m \hat{b}_j f(x_{n+1-j}, y_{n+1-j}),$$

in which the minimization is done both with respect to  $\hat{a}_i$ 's and  $\hat{b}_j$ 's is completely characterized by that it is locally interpolatory for the set of functions  $\{K(x, \bar{x}_{n+1-i}); i=1(1)m\} \cup \{D(x, \bar{x}_{n+1-j}); j = \delta_{to}(1)m\}$

### 1.6 Optimal Multistep Methods Interpolatory for Polynomials ( $\hat{M}^p$ )

For the purpose of derivation, a multistep method

$$Y_{n+1} = \sum_{i=1}^m a_i Y_{n+1-i} + h \sum_{j=\delta_{to}}^m b_j f(x_{n+1-j}, Y_{n+1-j})$$

can be written, using divided difference notation, as

$$(40) \quad Y_{n+1} = \sum_{i=1}^m a_i Y_{n+1-i} + h \sum_{j=\delta_{to}}^m \gamma_j Y' [x_{n+1-\delta_{to}}, x_{n-\delta_{to}}, \dots, x_{n+1-j}]$$

If  $p \leq m$  we can fix  $\{\gamma_j; j = \delta_{to}(1)p-1 + \delta_{to}\}$  in a manner that the method is exact for polynomial upto degree  $p$ .

Thus we have a formula

$$(41) \quad Y_{n+1} = \sum_{i=1}^m a_i Y_{n+1-i} + h \sum_{j=\delta_{to}}^{p-1+\delta_{to}} \gamma_j Y' [x_{n+1-\delta_{to}}, \dots, x_{n+1-j}] \\ = h \sum_{j=p+\delta_{to}}^m \gamma_j Y' [x_{n+1-\delta_{to}}, \dots, x_{n+1-j}],$$

in which the minimization of the norm of error is done with respect to  $\{\gamma_j; j = p+\delta_{to}(1)m\}$ .

If  $D(t, \bar{x})$  is the representer of the derivative evaluation, which is assumed to exist, then the representer of the

divided difference  $y'[x_{n+1-\delta_{t_0}}, \dots, x_{n+1-j}]$  is obviously

$$D[t; \bar{x}_{n+1-\delta_{t_0}}, \dots, \bar{x}_{n+1-j}],$$

which is obtained by having the divided difference of  $D(t, \bar{x})$  with respect to the second variable. This being simply a linear combination of  $D(t, \bar{x}_{n+1-\delta_{t_0}}) \dots D(t, \bar{x}_{n+1-j})$  involving constants, for any function  $f(t)$  we have

$$\begin{aligned} & (f(t), D[t; \bar{x}_{n+1-\delta_{t_0}}, \dots, \bar{x}_{n+1-j}]) \\ &= f'[x_{n+1-\delta_{t_0}}, \dots, x_{n+1-j}]; \end{aligned}$$

and therefore

$$\begin{aligned} p_{ij} &= (D[t; \bar{x}_{n+1-\delta_{t_0}}, \dots, \bar{x}_{n+1-i}], D[t; \bar{x}_{n+1-\delta_{t_0}}, \dots, \bar{x}_{n+1-j}]) \\ (42) \quad &= D'[x_{n+1-\delta_{t_0}}, \dots, x_{n+1-j}; \bar{x}_{n+1-\delta_{t_0}}, \dots, \bar{x}_{n+1-i}], \end{aligned}$$

which is the  $(i, j)$ th entry of the matrix obtained in the minimization of the norm of error in method given by (41).

Thus we can write the normal equations as

$$(43) \quad Px = q$$

where  $P$  is an  $(m-p-\delta_{t_0}+1) \times (m-p-\delta_{t_0}+1)$  matrix where  $p_{ij}$  are given by (42) and

$$\begin{aligned} q_i &= \frac{1}{h} \{ D[x_{n+1}; \bar{x}_{n+1-\delta_{t_0}}, \dots, \bar{x}_{n+1-i}] \\ (44) \quad & - \sum_{k=1}^m a_k D[x_{n+1-k}; \bar{x}_{n+1-\delta_{t_0}}, \dots, \bar{x}_{n+1-i}] \} \\ & - \sum_{l=\delta_{t_0}}^{p-1+\delta_{t_0}} \gamma_l D'[x_{n+1-\delta_{t_0}}, \dots, x_{n+1-l}; \bar{x}_{n+1-\delta_{t_0}}, \dots, \bar{x}_{n+1-i}] \end{aligned}$$

The matrix  $P$  is obtained by performing elementary row and column operations on a leading submatrix of the matrix of the linear system (37). Therefore  $P$  must be non-singular and thus the method (41) is also uniquely determined. By writing the representer of local truncation error for method (41) we can easily prove:

Theorem 6: A multistep method given by

$$Y_{n+1} = \sum_{i=1}^m a_i Y_{n+1-i} + h \sum_{j=\delta_{to}}^m \hat{b}_j f(x_{n+1-j}, Y_{n+1-j})$$

is optimal interpolatory for polynomials of degree  $p \leq m + \delta_{t1}$  if and only if it is interpolatory for the functions  $\{x^k; k=0(1)p\} \cup \{h_j; j=p+\delta_{to}(1)m\}$ , where

$$h_j = D[x; \bar{x}_{n+1-\delta_{to}}, \bar{x}_{n-\delta_{to}}, \dots, \bar{x}_{n+1-j}].$$

### 1.7 Optimal Multistep Methods Interpolatory for Arbitrary Functions ( $\hat{M}^F$ )

In this section we give a different approach for determining and characterizing a multistep method interpolatory for a set of arbitrary functions. (As compared to Section 1.4). The approach is based on Lagrangian multipliers. We first prove a result of general applicability:

Theorem 7: A necessary and sufficient condition that the multistep method given by

$$(45) \quad Y_{n+1} = \sum_{i=1}^m a_i Y_{n+1-i} + h \sum_{j=\delta_{to}}^m b_j f(x_{n+1-j}, Y_{n+1-j})$$

be interpolatory for functions  $f_1, f_2, \dots, f_p$  is that for every  $\varphi \in \text{span} \{f_1, \dots, f_p\}$  for which

$$\varphi'(x_{n+1-j}) = 0, \quad j = \delta_{t_0}(1)m$$

there holds

$$\varphi(x_{n+1}) = \sum_{i=1}^m a_i \varphi(x_{n+1-i})$$

Proof: The necessity part is obvious. For sufficiency assume that the stated conditions hold. Consider the system

$$(45) \quad \sum_{j=\delta_{t_0}}^m b_j f'_k(x_{n+1-j}) = f_k(x_{n+1}) - \sum_{i=1}^m a_i f_k(x_{n+1-i}), \quad k=1(1)p$$

of linear equations in  $b_j$ . Applying elementary row operations on the system (45) we can reduce it to one in which the matrix is in a row reduced echelon form. In this system the existence of a non-zero augmented entry corresponding to a zero row of the matrix would contradict the stated conditions. It follows that the system is consistent, completing the proof of the theorem.

In view of the above theorem and its proof, if a multi-step method interpolatory for  $\text{span} \{f_1, \dots, f_p\}$  is possible, there exist  $q \leq (m + \delta_{t_1})$  functions  $g_1, g_2, \dots, g_q$  in  $\text{span} \{f_1, \dots, f_p\}$  such that

$$(46) \quad \text{rank} \left[ g'_i(x_{n+1-j}) \right]_{\substack{i=1(1)q \\ j=\delta_{t_0}(1)m}} \leq q = \dim[\text{span} \{f_1, \dots, f_p\}]$$

and that the multistep method is interpolatory for span  $\{f_1, \dots, f_p\}$  if, and only if, it is interpolatory for  $g_1, g_2, \dots, g_q$ . Hence with preprocessing, if necessary, we can assume that  $f_1, \dots, f_p$  themselves are such that

$$(47) \quad \text{rank} \left[ f_k'(x_{n+1-j}) \right]_{\substack{k=1(1)p \\ j=\delta_{t0}(1)m}} = p \leq m + \delta_{t1}$$

Here in case  $p = m + \delta_{t1}$  all the coefficients  $b_j$ 's get uniquely determined and no optimization of error will be possible. Thus for optimal interpolatory methods we will assume that  $p < m + \delta_{t1}$  alongwith (47).

For an optimal method interpolatory for  $f_k \in \text{span} \{f_1, \dots, f_p\}$  we have

$$\|\hat{T}_n^F\| \text{ is minimum}$$

subject to

$$(48) \quad (\hat{T}_n^F, f_k) = 0, \quad k = 1(1)p,$$

where  $\hat{T}_n^F$  is the local truncation error functional corresponding to the method.

Equivalently we minimize

$$(49) \quad (\hat{T}_n^F, \hat{T}_n^F) + \sum_{k=1}^p \lambda_k (\hat{T}_n^F, f_k)$$

where  $\lambda_k$ 's are complex Lagrangian multipliers. Thus we have to minimize the quantity

$$\begin{aligned}
& (K(t, \bar{x}_{n+1}) - \sum_{i=1}^m \bar{a}_i K(t, \bar{x}_{n+1-i}) - h \sum_{j=\delta_{t0}}^m \bar{b}_j^F D(t, \bar{x}_{n+1-j}), \\
& K(t, \bar{x}_{n+1}) - \sum_{i=1}^m \bar{a}_i K(t, \bar{x}_{n+1-i}) - h \sum_{l=\delta_{t0}}^m \bar{b}_l^F D(t, \bar{x}_{n+1-l})) \\
& + \sum_{k=1}^p \lambda_k (K(t, \bar{x}_{n+1}) - \sum_{i=1}^m \bar{a}_i K(t, \bar{x}_{n+1-i}) \\
& - h \sum_{j=\delta_{t0}}^m \bar{b}_j^F D(t, \bar{x}_{n+1-j}), f_k),
\end{aligned}$$

giving rise to a system of linear equations

$$(50) \quad \begin{bmatrix} A & F^* \\ F & 0 \end{bmatrix} \begin{bmatrix} b \\ \lambda \end{bmatrix} = \begin{bmatrix} c \\ f \end{bmatrix}$$

where  $A$  is an  $(m + \delta_{t1}) \times (m + \delta_{t1})$  matrix with  $(i, j)$ th entry  $D'(x_{n+1-j}, \bar{x}_{n+1-i})$ ,  $F$  is  $p \times (m + \delta_{t1})$  matrix with  $(k, j)$ th entry as  $f'_k(x_{n+1-j})$ ,  $F^*$  is the adjoint of  $F$ ,  $0$  is a  $p \times p$  null matrix,

$$b = [\hat{b}_{\delta_{t0}}^F, \dots, \hat{b}_m^F]^T, \lambda = [\lambda_1, \dots, \lambda_p]^T, f = [f_1, \dots, f_p]^T$$

where 
$$f_k = f_k(x_{n+1}) - \sum_{i=1}^m \bar{a}_i f_k(x_{n+1-i})$$

and  $c = [c_{\delta_{t0}}, \dots, c_m]^T$ , where

$$\bar{c}_i = D(x_{n+1-i}, \bar{x}_{n+1}) - \sum_{j=1}^m \bar{a}_j D(x_{n+1-i}, \bar{x}_{n+1-j}).$$

If the rows of  $F$  are assumed to be linearly independent from that of  $A$  the system of linear equations can be solved

to have a unique solution.  $\hat{b}_j^F$ 's thus obtained will satisfy the required optimal interpolatory conditions. Now we characterize the optimal interpolatory multistep method  $\hat{M}^F$ .

For simplicity in the form of characterization we will assume that the last  $p$  columns in the matrix in (47) are linearly independent. (Note that in the general case some  $p$  columns of the matrix are linearly independent and in the corresponding characterization the indices of these columns instead of the last  $p$  columns in the simpler case would appear in the formulation.)

Let the interpolatory conditions appearing in (50) be rewritten as

$$[E|P] \begin{bmatrix} d \\ e \end{bmatrix} = f$$

where

$$E = [f_i^j(x_{n+1-j})]_{\substack{i=1(1)p \\ j=\delta_{to}(1)m-p}}$$

$$P = [f_i^j(x_{n+1-j})]_{\substack{i=1(1)p \\ j=m+1-p(1)m}}$$

$$d = [\hat{b}_{\delta_{to}}^F, \dots, \hat{b}_{m-p}^F]^T, \quad e = [\hat{b}_{m-p+1}^F, \dots, \hat{b}_m^F]^T \quad \text{and } f \text{ is}$$

as in (50). We get

$$e = P^{-1}(f - Ed) .$$

Let

$$(51) \quad r = P^{-1}f$$



and

$$(52) \quad G = P^{-1}E.$$

We have

$$(53) \quad e = r - Gd.$$

Then we can write

$$\begin{aligned}
 (54) \quad Y_{n+1} &= \sum_{i=1}^m a_i Y_{n+1-i} - h \sum_{j=\delta_{t_0}}^{m-p} \hat{b}_j^F Y'_{n+1-j} - h \sum_{j=m-p+1}^m \hat{b}_j^F Y'_{n+1-j} \\
 &= Y_{n+1} - \sum_{i=1}^m a_i Y_{n+1-i} - h \sum_{j=\delta_{t_0}}^{m-p} \hat{b}_j^F Y'_{n+1-j} \\
 &\quad - h \sum_{j=m-p+1}^m (r_{j-m+p} - \sum_{i=\delta_{t_0}}^{m-p} \hat{b}_i^F g_{j-m+p, i+1-\delta_{t_0}}) Y'_{n+1-j} \\
 &= \{ Y_{n+1} - \sum_{i=1}^m a_i Y_{n+1-i} - h \sum_{j=m-p+1}^m r_{j-m+p} Y'_{n+1-j} \} \\
 &\quad - h \sum_{j=\delta_{t_0}}^{m-p} \hat{b}_j^F \{ Y'_{n+1-j} + \sum_{i=m-p+1}^m g_{i-m+p, j-\delta_{t_0}+1} Y'_{n+1-j} \}.
 \end{aligned}$$

With the notations and assumptions as in the above the optimal interpolatory multistep method is characterized as follows:

Theorem 8: A multistep method given by

$$Y_{n+1} = \sum_{i=1}^m a_i Y_{n+1-i} + h \sum_{j=\delta_{t_0}}^m \hat{b}_j^F f(x_{n+1-j}, Y_{n+1-j}),$$

where the  $a_i$ 's are prefixed, is optimal interpolatory for

the functions  $f_1, f_2, \dots, f_p$  of (47) if, and only if, it is interpolatory for the functions

$$\{f_1, \dots, f_p\} \cup \{h_j : j = \delta_{t_0}(1)m-p\},$$

where for  $j = \delta_{t_0}(1)m-p$ ,

$$h_j = D(x, \bar{x}_{n+1-j}) + \sum_{i=m-p+1}^m \bar{g}_{i-m+p, j+1-\delta_{t_0}} D(x, \bar{x}_{n+1-i}),$$

$D(x, \bar{z})$  is the representer of the derivative evaluation functional at point  $\bar{z}$  and  $g$ 's are as in (52).

Proof: Equation (54) shows that to determine optimal coefficients  $(\hat{b}_j^F; j = \delta_{t_0}(1)m-p)$ , the normal equations may be obtained by minimizing the representer of (54) with respect to the coefficients  $\hat{b}_j^F, j = \delta_{t_0}(1)m-p$ .

Thus we obtain the equations

$$(h_j, \hat{T}_n^F) = 0, \quad j = \delta_{t_0}(1)m-p,$$

where

$$h_j = D(x, \bar{x}_{n+1-j}) + \sum_{i=m-p+1}^m \bar{g}_{i-m+p, j+1-\delta_{t_0}} D(x, \bar{x}_{n+1-i}).$$

As the method has been made interpolatory for functions  $\{f_1, f_2, \dots, f_p\}$  the proof is complete.

In Chapters 2 to 5 we have implemented the methods of this chapter in different situations. We present there the coefficients for 5 step methods with  $s = 0$  for the quadrature optimal case and  $a_1=1, a_2=a_3=a_4=a_5=0$  for

optimal case. Coefficients for non-interpolatory situation, interpolatory for polynomials upto degree 1 to 5 and interpolatory for  $\exp(\alpha x)$ ,  $\alpha = \pm 1.6$  have been calculated and presented in the form of tables for quadrature optimal and optimal case in the respective Hilbert spaces. Coefficients have been obtained for the interval  $[-2.0, 2.0]$  with step size  $h = .1$  and equispaced points. All the methods have been applied for a set of twenty four differential equations by providing exact starting values (calculated from the analytical solutions) at 5 points prior to  $-1.2$ . The solutions have been computed on the interval  $[-1.2, 1.2]$  and compared with usual 5 step methods.

The twenty four equations and the analytical (particular) solutions are as follows:

$$1. \quad \frac{dy}{dx} = xy^3 ; y = (2.01^2 - x^2)^{-1/2}$$

$$2. \quad \frac{dy}{dx} = xy^3 ; y = (2.11^2 - x^2)^{-1/2}$$

$$3. \quad \frac{dy}{dx} = 2xy^2 ; y = (2.03^2 - x^2)^{-1}$$

$$4. \quad \frac{dy}{dx} = 2xy^2 ; y = (2.11^2 - x^2)^{-1}$$

$$5. \quad \frac{dy}{dx} = -2xe^{-y} ; y = \log(2.01^2 - x^2)$$

$$6. \quad \frac{dy}{dx} = 4x^3 y^2 ; y = (2.01^4 - x^4)^{-1}$$

$$7. \quad \frac{dy}{dx} = 6x^5 y^2 ; y = (2.01^6 - x^6)^{-1}$$

$$8. \quad \frac{dy}{dx} = 2x^3 y^3 ; y = (2.01^4 - x^4)^{-1/2}$$

$$9. \quad \frac{dy}{dx} = 3x^5 y^3 ; y = (2.01^6 - x^6)^{-1/2}$$

$$10. \quad \frac{dy}{dx} = 2xy ; y = e^{x^2}$$

$$11. \quad \frac{dy}{dx} = 3(y - e^{-3x}) ; y = \cosh(3x)$$

$$12. \quad \frac{dy}{dx} = 3(y + e^{-3x}) ; y = \sinh(3x)$$

$$13. \quad \frac{dy}{dx} = xy^3 ; y = (2.75^2 - x^2)^{-1/2}$$

$$14. \quad \frac{dy}{dx} = xy^3 ; y = (2.85^2 - x^2)^{-1/2}$$

$$15. \quad \frac{dy}{dx} = 2xy^2 ; y = (2.77^2 - x^2)^{-1}$$

$$16. \quad \frac{dy}{dx} = 2xy^2 ; y = (2.85^2 - x^2)^{-1}$$

$$17. \quad \frac{dy}{dx} = 6x^5 y^2 ; y = (2.85^6 - x^6)^{-1}$$

$$18. \quad \frac{dy}{dx} = 3x^5 y^3 ; y = (2.9^6 - x^6)^{-1/2}$$

$$19. \quad \frac{dy}{dx} = 2x(y^2 - \frac{2y}{x^2 + .9}) ; y = (2.02^2 - x^2)^{-1} + (x^2 + .9)^{-1}$$

$$20. \quad \frac{dy}{dx} = 2xy^2(2x^2 - 3.1804) ; y = (2.02^2 - x^2)^{-1} (x^2 + .9)^{-1}$$

$$21. \quad \frac{dy}{dx} = xy^3(2x^2 - 3.1804) ; y = (2.02^2 - x^2)(x + .9)^{-1/2}$$

$$22. \quad \frac{dy}{dx} = x \left\{ (y - \frac{1}{\sqrt{x^2 + .9}})^3 - (\frac{1}{\sqrt{x^2 + .9}})^3 \right\} ; y = (2.02^2 - x^2)^{-1/2} + (x^2 + .9)^{-1/2}$$

$$23. \quad \frac{dy}{dx} = - \frac{2x(e^{-y} + 1)}{x^2 + .9} ; y = \log \left( \frac{2.02^2 - x^2}{x^2 + .9} \right)$$

$$24. \quad \frac{dy}{dx} = 3x^5 y^3 (x^2 + .9)^2 - \frac{2xy}{x^2 + .9} ; y = \frac{(2.02^6 - x^6)^{-1/2}}{x^2 + .9}$$

The first nine of the solutions have singularities of various types near the boundary of the domain of the Hilbert spaces that would be considered in chapters 2-5. The solutions ~~of next three~~ equations 10-12 are entire functions of rather fast growth. The solutions corresponding to equations 13-18 have singularities comparatively far remote from the domain of the underlying spaces. The last six equations have solutions with singularities inside the domain. Thus through these twenty four cases we have tried to cover most of the important theoretical situations that arise in the case of analytic solutions.

## CHAPTER 2

### QUADRATURE OPTIMAL MULTISTEP METHODS IN $H^2(c_r)$

#### 2.1 Introduction

Quadrature formulae of various types for functions in the space  $H^2(c_r)$  have been studied by Larkin [32], Richter [39], [40], [41], Chawla and Kaul [16], [17], [18], Finney and Price Jr [24] and others. The methods involve choosing the coefficients and/or nodes to minimize the norm of error without or with some constraints. The results of these authors show that the error in the quadrature formulae optimized over  $H^2(c_r)$  is substantially smaller than that corresponding to classical quadrature rules. In this chapter we consider the applicability of such optimal quadrature rules in  $H^2(c_r)$  to initial value problem for first order differential equations.

For the purpose of numerical illustration we have worked with quadrature optimal multistep methods of Adams-Bashforth and Adams-Moulton type.

In Section 2.2 we describe the space  $H^2(c_r)$  and establish the boundedness of derivative evaluation functional of any order at a point inside  $c_r$ . In Section 2.3 we present the construction of quadrature optimal

methods in  $H^2(c_r)$  and some numerical results obtained on applying the method of 5-step on differential equations. The coefficients and norms of local truncation error functionals of implicit and explicit 5 step methods for  $h = 0.1$  and the results obtained by applying these to differential equations are given and compared with the corresponding usual methods. In Section 2.4 we describe the quadrature optimal multistep methods of 5 steps interpolatory for polynomials of degree one to five. The coefficients and local truncation error functional norms are given in tabular form and behaviour on the differential equations is described. In Section 2.5 we present quadrature optimal multistep methods of 5-step interpolatory for a set of selected functions. In Section 2.6 we discuss the behaviour of the coefficients of quadrature optimal multistep methods in  $H^2(c_r)$  as  $r \rightarrow \infty$ . In Section 2.7 a comparison of different methods is presented.

## 2.2 The Hilbert Space $H^2(c_r)$

The space  $H^2(c_r)$  consists of analytic functions regular in the disk  $D_r = \{z : |z| < r\}$  with the magnitude of boundary values square integrable on the circle  $c_r = \{z : |z| = r\}$ . The space  $H^2(c_r)$  is a Hilbert space with the inner product defined by

$$(1) \quad (f, g) = \int_{c_r} f(z) \overline{g(z)} \, ds, \quad f, g \in H^2(c_r),$$

the integration being with respect to the length element on the circle. The space possesses a reproducing kernel function given by

$$(2) \quad K(z, \bar{t}) = \frac{r}{2\pi(r^2 - z\bar{t})}$$

and a complete orthonormal sequence  $\{\Psi_k\}$  of functions ([43])

$$(3) \quad \Psi_k(z) = \frac{z^k}{\sqrt{2\pi}r} r^k, \quad k=0,1,2,\dots$$

By virtue of the space  $H^2(c_r)$  possessing a reproducing kernel function the point evaluation functional

$$L_z: f(\epsilon H^2(c_r)) \rightarrow f(z), \quad (z \in D_r),$$

is a bounded linear functional on  $H^2(c_r)$ . In the sequel we require the boundedness of the derivative evaluation functional of order  $k$

$$D_z^k: f(\epsilon H^2(c_r)) \rightarrow f^{(k)}(z) \quad (z \in D_r),$$

where  $k$  is a positive integer:

Theorem 1: For  $z \in D_r$  and  $k$  any positive integer  $D_z^k$  is a bounded linear functional in  $H^2(c_r)$  with

$$(5) \quad \|D^k(z)\| \leq \frac{k! \sqrt{r}}{\sqrt{2\pi}(r-|z|)^{k+1}}.$$

Proof: Using Cauchy integral formula, if  $\delta$  denotes the distance of a point  $z \in D_r$  from  $c_r$ , we have



$$\begin{aligned}
|f^{(k)}(z)| &\leq \frac{k!}{2\pi} \int_{c_r} \frac{|f(w)|}{|w-z|^{k+1}} |dw| \\
&\leq \frac{k!}{2\pi \delta^{k+1}} \int_{c_r} |f(w)| |dw| \\
&\leq \left(\frac{r}{2\pi}\right)^{1/2} \frac{k!}{\delta^{k+1}} \|f\|,
\end{aligned}$$

by Cauchy-Schwarz inequality. From this the result is immediate.

That the operation of evaluating a definite integral corresponds to a bounded linear functional in  $H^2(c_r)$  is well known (e.g. Larkin [32]) moreover we have

$$(6) \quad \int_{z_1}^{z_2} f(z) dz = (f(t), \frac{r}{2\pi t} \log \left( \frac{r^2 - t\bar{z}_1}{r^2 - t\bar{z}_2} \right)), f \in H^2(c_r)$$

showing that the representer  $l_{(z_1, z_2)}(t)$  of the definite integral functional is given by

$$(7) \quad l_{(z_1, z_2)}(t) = \frac{r}{2\pi t} \log \left( \frac{r^2 - t\bar{z}_1}{r^2 - t\bar{z}_2} \right).$$

### 2.3 Quadrature Optimal Multistep Method in $H^2(c_r)$

For determining the coefficients of a quadrature optimal multistep formula

$$(8) \quad Y_{n+1} = Y_{n-s} + h \sum_{j=\delta_{to}}^m \tilde{b}_j f(x_{n+1-j}, Y_{n+1-j})$$

in  $H^2(c_r)$  we use the equations (1.6) (equation (6) of Chapter 1), (2) and (7). Thus we have the normal equations

$$(9) \quad \tilde{C} \tilde{b} = \tilde{d}$$

with

$$c_{ij}^z = \frac{r}{2\pi(r^2 - x_{n+1-j} \bar{x}_{n+1-i})}$$

and

$$d_i^z = \begin{cases} \frac{r}{2\pi h \bar{x}_{n+1-i}} \log \left( \frac{r^2 - x_{n-s} \bar{x}_{n+1-i}}{r^2 - x_{n+1} \bar{x}_{n+1-i}} \right), & \text{if } x_{n+1-i} \neq 0 \\ \frac{x_{n+1} - x_n}{2\pi r h}, & \text{if } x_{n+1-i} = 0, i, j = \delta_{t_0}(1)m \end{cases}$$

Equations given by (9) can be solved analytically as follows:

We know that

$$(10) \det(\tilde{C}) = r^k \frac{\prod_{m \geq i > j \geq \delta_{t_0}} (x_{n+1-i} - x_{n+1-j})(\bar{x}_{n+1-i} - \bar{x}_{n+1-j})}{\prod_{i=\delta_{t_0}}^m \prod_{j=\delta_{t_0}}^m (r^2 - x_{n+1-i} \bar{x}_{n+1-j})},$$

where

$$k = (m + \delta_{t_1})(m + \delta_{t_1} - 1),$$

and

$$M = \left(\frac{r}{2\pi}\right)^{m + \delta_{t_1}}.$$

Using Cramer's rule we get  $\tilde{C}^{-1} = G$ , (say), where for  $l, k = \delta_{t_0}(1)m$

$$g_{lk} = \left(\frac{r}{2\pi}\right)^{-1} \frac{\prod_{j=\delta_{t_0}}^m (r^2 - x_{n+1-k} \bar{x}_{n+1-j}) \prod_{i=\delta_{t_0}}^m (r^2 - x_{n+1-i} \bar{x}_{n+1-l})}{r^{2(m + \delta_{t_1})} (r^2 - x_{n+1-k} \bar{x}_{n+1-l}) \prod_{\substack{j=\delta_{t_0} \\ j \neq k}}^m (x_{n+1-k} - x_{n+1-j}) \cdot \prod_{\substack{i=\delta_{t_0} \\ i \neq k}}^m (\bar{x}_{n+1-l} - \bar{x}_{n+1-i})}.$$

Therefore, the coefficients are given by

$$b_l = \frac{1}{h} \sum_{k=\delta_{to}}^m g_{lk} \frac{r}{2\pi h} \left\{ \frac{1}{\bar{x}_{n+1-k}} \log \left( \frac{r^{2-x_n-s} \bar{x}_{n+1-k}}{r^{2-x_{n+1}} \bar{x}_{n+1-k}} \right) \right\}^*, \quad l=\delta_{to}(1)m,$$

$\{.\}^*$  denoting limiting value if  $x_{n+1-k} = 0$ .

Thus the method (8) gets determined explicitly.

In view of Theorem 1.1 (Theorem p q denotes qth theorem of Chapter p) we have

Theorem 2: The quadrature optimal multistep formula (8) in  $H^2(c_r)$  is characterized by that it is locally interpolatory for functions

$$y_i(x) = \begin{cases} \log(r^{2-x} \bar{x}_{n+1-i}) & , \text{ if } x_{n+1-i} \neq 0 \\ x & , \text{ if } x_{n+1-i} = 0, i = \delta_{to}(1)m. \end{cases}$$

Proof: From (2), (7) and Theorem 1.1 it follows that the formula (8) is interpolatory for functions

$$g_i(x) = \begin{cases} \frac{r}{2\pi \bar{x}_{n+1-i}} \log(r^{2-x} \bar{x}_{n+1-i}) & , \text{ if } x_{n+1-i} \neq 0 \\ \frac{x}{2\pi r} & , \text{ if } x_{n+1-i} = 0, i = \delta_{to}(1)m. \end{cases}$$

Suppressing the scalar multipliers in  $g_i(x)$  we get the result.

From this theorem we note that if  $x_{n+1-i} = 0$  for some  $i$  with  $\delta_{to} \leq i \leq m$ , i.e. the origin is a node used in the quadrature optimal multistep formula, it becomes exact for polynomials of degree 1.

In Table 2.1 we present the norms of local truncation error functionals and the coefficients of explicit and implicit quadrature optimal 5-step method in  $H^2(C_r)$  with  $s=0$ . The norm of local truncation error for 5-step usual methods is also given at each point. The norms of local truncation error functionals as defined in equation (1.7) (equation 7 of Chapter 1) may be calculated by using the following:

For any coefficients  $b_j$ ,  $j=\delta_{to}(1)m$  the norm of the local truncation error functional  $T_n$  at  $x_{n+1}$  is given by

$$\begin{aligned}
 \|T_n\|^2 = & \frac{r}{2\pi} \left[ \frac{1}{r^2 - |x_{n+1}|^2} + \frac{1}{r^2 - |x_{n-s}|^2} - 2 \operatorname{Re} \left( \frac{1}{r^2 - x_{n+1} \bar{x}_{n-s}} \right) \right. \\
 (11) \quad & - h \sum_{j=\delta_{to}}^m b_j g(x_{n+1-j}) - h \sum_{k=\delta_{to}}^m \bar{b}_k \overline{g(x_{n+1-k})} - \\
 & \left. - h \sum_{j=\delta_{to}}^m b_j \frac{r^2 + x_{n+1-j} \bar{x}_{n+1-k}}{(r^2 - x_{n+1-j} \bar{x}_{n+1-k})^3} \right] ,
 \end{aligned}$$

where

$$g(x) = x[(r^2 - \bar{x}_{n+1}x)^{-2} - (r^2 - \bar{x}_{n-s}x)^{-2}] ,$$

Here  $\operatorname{Re}(\cdot)$  denotes the real part of the quantity.

All the computations were carried out on DEC-1090 computer system of the Institute. The coefficients (which have been obtained by Gaussian method for the system of linear equations) and the norms of the error functionals

were computed using double precision, while the solutions of the differential equations were obtained using single precision. All through the thesis the computations are confined to the interval  $[-2, 2]$ , a real situation. We have taken  $r = 2.01$  &  $h = 0.1$ . The interval on which any formula is applied is  $[-1.2, 1.2]$  (by providing true values of the solution at the five points  $-1.7, -1.6, -1.5, -1.4$  and  $-1.3$ ). Implicit formulae in all cases have been implemented by providing initial approximation generated by an application of the explicit formula of corresponding type on the last five values obtained by the implicit method (or the exact values at the beginning). Iterations were carried out till the difference of two consecutive iterates was smaller than  $1 \times 10^{-8}$  in absolute value, subject to a maximum of ten iterations.

From Table 2.1 we observe, in both implicit and explicit cases, that at  $x = -1.5$  the norm of local truncation error functional for usual formula is more than a thousand times the corresponding norm for quadrature optimal formula. In central region (around  $x = 0.2, 0.3$ ) the norm of local truncation error functionals of the usual and quadrature optimal formulae are almost same. From here onwards again the error functional norms for the usual formulae start becoming larger than those of the quadrature optimal formulae.

Table 2.1

[illegible]

Table 2.1(a)

[illegible]

Table 2.1(b)

[illegible]



Table 2.1(c)

[illegible]

Table 2.1(d)

[illegible]

From Table 2.1 we also see that the coefficients of the  $H^2(c_r)$ -quadrature optimal methods vary from point to point. It is interesting to note that the magnitude of each of the coefficients, however, is an increasing function of  $x$  except the first coefficient of implicit method which decreases with  $x$ . Moreover in the central region the coefficients approximately equal the usual coefficients.

Following Table 2.1, in Tables 2.1(a)-2.1(d) we present numerical results obtained by using the coefficients of Table 2.1 and the usual coefficients on the twenty four differential equations (given at the end of Chapter 1).

From Tables 2.1(a)-2.1(d) it is clear that the  $H^2(c_r)$ -quadrature optimal 5-step methods have performed better than the corresponding usual methods which turn out to be the Adams-Bashforth/Adams-Moulton 5-step methods (for  $s=0$ ). The explicit method has been just better on equations 13, 14 and 24 one decimal place more accurate on equations 2, 3, 6, 8, 9, 10, 11, 15, 16, 17, 18, 19, and 23 ; and two decimal places on equations 1, 4, 5, 7, 12, 20, 21 and 22. The implicit quadrature optimal method is found just better on equations 17 and 18; one decimal place better on equations 7, 11, 12, 13, 14, 15, 16, 19, 20, 21, 22, 23 and 24; and two decimal places on equations 1, 2, 3, 4, 5, 6, 8, 9, and 10. We also observe that the full 10 iterations were carried out rarely. Indeed, in this work idea has been only to check the effectiveness

of the basic implicit scheme. In actual practice, of course, one would utilize a more appropriate predictor corrector scheme.

## 2.4 Quadrature Optimal Multistep Methods in $H^2(c_r)$ Interpolatory for Polynomials

In Chapter 1 we have given an approach for determining quadrature optimal multistep methods interpolatory for polynomials in a general set up. Here we specialize the case when the points  $x_{n+1-i}$ 's lie along a straight line in  $D_r$ , the consecutive points equispaced with distance  $h$ . It is obvious that

$$(12) \quad y_{n+1} = y_{n-s} + h \sum_{j=0}^{m-\delta_{t0}} \gamma_j \nabla^j f(x_{n+\delta_{t1}}, y_{n+\delta_{t1}})$$

represents a general  $m$  step method of quadrature type. From this it follows that a general method interpolatory for polynomials of degree  $p < m + \delta_{t1}$  may be written as

$$(13) \quad y_{n+1} - y_{n-s} - h \sum_{j=0}^{p-1} \gamma_j^u \nabla^j f(x_{n+\delta_{t1}}, y_{n+\delta_{t1}}) \\ = h \sum_{j=p}^{m-\delta_{t0}} \gamma_j \nabla^j f(x_{n+\delta_{t1}}, y_{n+\delta_{t1}}),$$

where the coefficients  $\gamma_j^u$ 's are defined as in the corresponding usual formula. In a quadrature optimal multistep formula interpolatory for polynomials of degree  $p$ , the remaining coefficients  $\gamma_j$ ,  $j=p(1)m-\delta_{t0}$

are to be determined by minimization of the norm of the quadrature error functional over the space  $H^2(c_r)$ .

Proceeding as in Section 1.6 it follows that the unknown  $\gamma_j$ 's are to satisfy the normal equations

$$(14) \quad \tilde{C}^p \tilde{\gamma}^p = \tilde{d}^p,$$

where

$$\tilde{\gamma}^p = (\gamma_p, \dots, \gamma_{m-\delta_{t0}})^T,$$

$$\tilde{C}_{ij}^p = \frac{r}{2\pi} \sum_{k=0}^j \sum_{l=0}^i (-1)^{l+k} \binom{i}{l} \binom{j}{k} r^{2-x_{n+\delta_{t1}}-k} \bar{x}_{n+\delta_{t1}}^{l-1},$$

and

$$\begin{aligned} \tilde{d}_i^p = & \frac{r}{2\pi h} \left[ \sum_{l=0}^i (-1)^l \binom{i}{l} \left\{ \frac{1}{\bar{x}_{n+\delta_{t1}}^{l-1}} \log \left( \frac{r^{2-x_{n-s}} \bar{x}_{n+\delta_{t1}}^{l-1}}{r^{2-x_{n+1}} \bar{x}_{n+\delta_{t1}}^{l-1}} \right) \right\}^* \right] \\ & - \frac{r}{2\pi} \sum_{q=0}^{p-1} \gamma_q^u \left( \sum_{k=0}^q \sum_{l=0}^i (-1)^{l+k} \binom{i}{l} \binom{q}{k} \frac{1}{r^{2-x_{n+\delta_{t1}}-k} \bar{x}_{n+\delta_{t1}}^{l-1}} \right), \end{aligned}$$

$$i, j = p(1)m - \delta_{t0}.$$

Here  $(x_{n+1} - x_{n-s})/r^2$  replaces  $\{.\}^*$  if  $x_{n+\delta_{t1}} - 1 = 0$ .

The multistep coefficients  $\tilde{b}_i^p$  (as in (1.8)) can then be calculated as in the usual case.

Theorem 3: In  $H^2(c_r)$ , a quadrature optimal multistep method

(13) interpolatory for polynomials of degree  $p < m + \delta_{t1}$  is

characterized by that it is locally interpolatory for

functions  $\{x^j; 1 \leq j \leq p\} \cup \{h_j(x); j = p(1)m - \delta_{t0}\}$  with

$$h_j(x) = \sum_{k=0}^j (-1)^{k+1} \binom{j}{k} \left\{ \frac{1}{\bar{x}_{n+\delta_{t1}-k}} \log (r^2 - x \bar{x}_{n+\delta_{t1}-k}) \right\}^*,$$

where \* indicates that if  $\bar{x}_{n+\delta_{t1}-k} = 0$ , the expression within the brackets is to be replaced by  $x/r^2$ .

Proof: The result is immediate from (14) along the lines of Theorem 2.

In Tables 2.2 through 2.6 we present the coefficients and error norms for  $H^2(c_r)$ -quadrature optimal 5-step methods interpolatory for polynomials of degree  $p = 1(1)5$ . For the comparison purpose, error norms of the corresponding usual methods have also been included. While going through Tables 2.2 to 2.6 we observe that the error norm for quadrature optimal method starts increasing when the interpolatory conditions are increased. In Table 2.6, where the polynomial precision is 5, the explicit method has become the usual method.

As the quadrature optimal multistep methods interpolatory for polynomials of degree  $p = 1(1)5$  have performed more or less in between the optimal and the usual methods we do not include complete tables of the results obtained by applying these methods on the differential equations. However a summary of the results observed is as follows:

The  $H^2(c_r)$ -explicit quadrature optimal multistep method with  $p=1$  has been just better on equations 13, 14,

[illegible][illegible]





SITUATION: Y' IN H (C r) R= 2.01 H= 10

MULTI STEP METHOD OF 5 STEPS INTERPOLATRY UPTO 3 DEGREE POLYNOMIALS

X	EUSUAL	EUPTUAL	H X B(1)	H X B(2)	H X B(3)	H X B(4)	H X B(5)
-1.50	0.60	0.70	0.20	0.16	0.73	0.10	0.29
-1.40	0.60	0.70	0.21	0.16	0.73	0.10	0.29
-1.30	0.60	0.70	0.22	0.16	0.73	0.10	0.29
-1.20	0.60	0.70	0.23	0.16	0.73	0.10	0.29
-1.10	0.60	0.70	0.24	0.16	0.73	0.10	0.29
-1.00	0.60	0.70	0.25	0.16	0.73	0.10	0.29
-0.90	0.60	0.70	0.26	0.16	0.73	0.10	0.29
-0.80	0.60	0.70	0.27	0.16	0.73	0.10	0.29
-0.70	0.60	0.70	0.28	0.16	0.73	0.10	0.29
-0.60	0.60	0.70	0.29	0.16	0.73	0.10	0.29
-0.50	0.60	0.70	0.30	0.16	0.73	0.10	0.29
-0.40	0.60	0.70	0.31	0.16	0.73	0.10	0.29
-0.30	0.60	0.70	0.32	0.16	0.73	0.10	0.29
-0.20	0.60	0.70	0.33	0.16	0.73	0.10	0.29
-0.10	0.60	0.70	0.34	0.16	0.73	0.10	0.29
0.00	0.60	0.70	0.35	0.16	0.73	0.10	0.29
0.10	0.60	0.70	0.36	0.16	0.73	0.10	0.29
0.20	0.60	0.70	0.37	0.16	0.73	0.10	0.29
0.30	0.60	0.70	0.38	0.16	0.73	0.10	0.29
0.40	0.60	0.70	0.39	0.16	0.73	0.10	0.29
0.50	0.60	0.70	0.40	0.16	0.73	0.10	0.29
0.60	0.60	0.70	0.41	0.16	0.73	0.10	0.29
0.70	0.60	0.70	0.42	0.16	0.73	0.10	0.29
0.80	0.60	0.70	0.43	0.16	0.73	0.10	0.29
0.90	0.60	0.70	0.44	0.16	0.73	0.10	0.29
1.00	0.60	0.70	0.45	0.16	0.73	0.10	0.29
1.10	0.60	0.70	0.46	0.16	0.73	0.10	0.29
1.20	0.60	0.70	0.47	0.16	0.73	0.10	0.29
1.30	0.60	0.70	0.48	0.16	0.73	0.10	0.29
1.40	0.60	0.70	0.49	0.16	0.73	0.10	0.29
1.50	0.60	0.70	0.50	0.16	0.73	0.10	0.29

X	EUSUAL	EUPTUAL	H X B(1)	H X B(2)	H X B(3)	H X B(4)	H X B(5)
-1.50	0.60	0.70	0.20	0.16	0.73	0.10	0.29
-1.40	0.60	0.70	0.21	0.16	0.73	0.10	0.29
-1.30	0.60	0.70	0.22	0.16	0.73	0.10	0.29
-1.20	0.60	0.70	0.23	0.16	0.73	0.10	0.29
-1.10	0.60	0.70	0.24	0.16	0.73	0.10	0.29
-1.00	0.60	0.70	0.25	0.16	0.73	0.10	0.29
-0.90	0.60	0.70	0.26	0.16	0.73	0.10	0.29
-0.80	0.60	0.70	0.27	0.16	0.73	0.10	0.29
-0.70	0.60	0.70	0.28	0.16	0.73	0.10	0.29
-0.60	0.60	0.70	0.29	0.16	0.73	0.10	0.29
-0.50	0.60	0.70	0.30	0.16	0.73	0.10	0.29
-0.40	0.60	0.70	0.31	0.16	0.73	0.10	0.29
-0.30	0.60	0.70	0.32	0.16	0.73	0.10	0.29
-0.20	0.60	0.70	0.33	0.16	0.73	0.10	0.29
-0.10	0.60	0.70	0.34	0.16	0.73	0.10	0.29
0.00	0.60	0.70	0.35	0.16	0.73	0.10	0.29
0.10	0.60	0.70	0.36	0.16	0.73	0.10	0.29
0.20	0.60	0.70	0.37	0.16	0.73	0.10	0.29
0.30	0.60	0.70	0.38	0.16	0.73	0.10	0.29
0.40	0.60	0.70	0.39	0.16	0.73	0.10	0.29
0.50	0.60	0.70	0.40	0.16	0.73	0.10	0.29
0.60	0.60	0.70	0.41	0.16	0.73	0.10	0.29
0.70	0.60	0.70	0.42	0.16	0.73	0.10	0.29
0.80	0.60	0.70	0.43	0.16	0.73	0.10	0.29
0.90	0.60	0.70	0.44	0.16	0.73	0.10	0.29
1.00	0.60	0.70	0.45	0.16	0.73	0.10	0.29
1.10	0.60	0.70	0.46	0.16	0.73	0.10	0.29
1.20	0.60	0.70	0.47	0.16	0.73	0.10	0.29
1.30	0.60	0.70	0.48	0.16	0.73	0.10	0.29
1.40	0.60	0.70	0.49	0.16	0.73	0.10	0.29
1.50	0.60	0.70	0.50	0.16	0.73	0.10	0.29

Table 2.5

SITUATION:  $Y'$  IN  $H(C, r)$ ;  $R = 2.01$ ;  $H = 10$ 

MULTI STEP METHOD OF 5 STEPS INTERPOLATRY UPTO 4 DEGREE POLYNOMIALS

X	EUSUAL	OPTIMAL	H X B(1)	H X B(2)	H X B(3)	H X B(4)	H X B(5)
-1.50	0.670+01	0.160+00	0.2296717D+00	-0.24903534D+00	0.15959680D+00	0.4702010D-01	0.0050250-03
-1.40	0.690+00	0.940-02	0.2235064D+00	-0.24903534D+00	0.15959680D+00	0.4702010D-01	0.0050250-03
-1.30	0.910+02	0.247489D+00	0.2235064D+00	-0.24903534D+00	0.15959680D+00	0.4702010D-01	0.0050250-03
-1.20	0.210+02	0.190-03	0.2235064D+00	-0.24903534D+00	0.15959680D+00	0.4702010D-01	0.0050250-03
-1.10	0.670+03	0.247489D+00	0.2235064D+00	-0.24903534D+00	0.15959680D+00	0.4702010D-01	0.0050250-03
-1.00	0.260+03	0.170-04	0.2235064D+00	-0.24903534D+00	0.15959680D+00	0.4702010D-01	0.0050250-03
-0.90	0.510+03	0.180-04	0.2235064D+00	-0.24903534D+00	0.15959680D+00	0.4702010D-01	0.0050250-03
-0.80	0.550+03	0.180-04	0.2235064D+00	-0.24903534D+00	0.15959680D+00	0.4702010D-01	0.0050250-03
-0.70	0.720+03	0.180-04	0.2235064D+00	-0.24903534D+00	0.15959680D+00	0.4702010D-01	0.0050250-03
-0.60	0.210+03	0.180-04	0.2235064D+00	-0.24903534D+00	0.15959680D+00	0.4702010D-01	0.0050250-03
-0.50	0.210+03	0.180-04	0.2235064D+00	-0.24903534D+00	0.15959680D+00	0.4702010D-01	0.0050250-03
-0.40	0.210+03	0.180-04	0.2235064D+00	-0.24903534D+00	0.15959680D+00	0.4702010D-01	0.0050250-03
-0.30	0.210+03	0.180-04	0.2235064D+00	-0.24903534D+00	0.15959680D+00	0.4702010D-01	0.0050250-03
-0.20	0.210+03	0.180-04	0.2235064D+00	-0.24903534D+00	0.15959680D+00	0.4702010D-01	0.0050250-03
-0.10	0.210+03	0.180-04	0.2235064D+00	-0.24903534D+00	0.15959680D+00	0.4702010D-01	0.0050250-03
0.00	0.210+03	0.180-04	0.2235064D+00	-0.24903534D+00	0.15959680D+00	0.4702010D-01	0.0050250-03
0.10	0.210+03	0.180-04	0.2235064D+00	-0.24903534D+00	0.15959680D+00	0.4702010D-01	0.0050250-03
0.20	0.210+03	0.180-04	0.2235064D+00	-0.24903534D+00	0.15959680D+00	0.4702010D-01	0.0050250-03
0.30	0.210+03	0.180-04	0.2235064D+00	-0.24903534D+00	0.15959680D+00	0.4702010D-01	0.0050250-03
0.40	0.210+03	0.180-04	0.2235064D+00	-0.24903534D+00	0.15959680D+00	0.4702010D-01	0.0050250-03
0.50	0.210+03	0.180-04	0.2235064D+00	-0.24903534D+00	0.15959680D+00	0.4702010D-01	0.0050250-03
0.60	0.210+03	0.180-04	0.2235064D+00	-0.24903534D+00	0.15959680D+00	0.4702010D-01	0.0050250-03
0.70	0.210+03	0.180-04	0.2235064D+00	-0.24903534D+00	0.15959680D+00	0.4702010D-01	0.0050250-03
0.80	0.210+03	0.180-04	0.2235064D+00	-0.24903534D+00	0.15959680D+00	0.4702010D-01	0.0050250-03
0.90	0.210+03	0.180-04	0.2235064D+00	-0.24903534D+00	0.15959680D+00	0.4702010D-01	0.0050250-03
1.00	0.210+03	0.180-04	0.2235064D+00	-0.24903534D+00	0.15959680D+00	0.4702010D-01	0.0050250-03
1.10	0.210+03	0.180-04	0.2235064D+00	-0.24903534D+00	0.15959680D+00	0.4702010D-01	0.0050250-03
1.20	0.210+03	0.180-04	0.2235064D+00	-0.24903534D+00	0.15959680D+00	0.4702010D-01	0.0050250-03
1.30	0.210+03	0.180-04	0.2235064D+00	-0.24903534D+00	0.15959680D+00	0.4702010D-01	0.0050250-03
1.40	0.210+03	0.180-04	0.2235064D+00	-0.24903534D+00	0.15959680D+00	0.4702010D-01	0.0050250-03
1.50	0.210+03	0.180-04	0.2235064D+00	-0.24903534D+00	0.15959680D+00	0.4702010D-01	0.0050250-03

Table 7.6

$$2 \nu_{\text{H}}(C_1) \cdot D = 2.01 \text{ H} = 10$$

SITUATION: Y' IN H(C, r); R = 2.01 H = 10  
UNIT: STEP METHOD OF 5 STEPS; INTERPOLATED Y UPTO 5 DEGREE POLYNOMIALS

MULTI STEP METHOD OF 5 STEPS INTERPOLATION OF 3 DEGREE POLYNOMIALS

[illegible]

16 and 24; one decimal place better on equations 2,3,6,8, 9,10,11,12,15,17,18,19 and 23; and two places better on equations 1,4,5,7,20,21, and 22. The implicit method with  $p=1$  is found just better on equations 17 and 18; one decimal place better on equations 7,11,12,13,14,15,16,19,20,21,22,23 and 24; and two decimal places better on equations 1,2,3,4, 5,6,8,9 and 10.

The explicit method with  $p=2$  has been just better on equation 24; one decimal place better on equations 2,3,6,8, 9,10,11,12,13,14,16,17,18,19 and 23; and two decimal places better on equations 1,4,5,7,15,20,21 and 22. The implicit method with  $p=2$  was just better on equations 17 and 18; one decimal place better on equations 1,5,7,11,12,13,14,19, 20,21,22,23 and 24; and two decimal places better on equations 2,3,4,6,8,9,10,15 and 16.

The explicit method with  $p=3$  is found just better on equations 11,12,14,16,17,18 and 24; one decimal place better on equations 1,2,3,4,5,6,7,8,9,10,13,15,19,20 and 23; and two decimal places better on equation 21. The implicit method with  $p=3$  has been just better on equations 11,12, 17,18 and 24; one decimal place better on equations 1,3,5, 7,13,14,15,16,19,20,21,22 and 23; and two decimal places better on equations 2,4,6,8,9 and 10.

The explicit method with  $p=4$  was just better on equations 6,14,16,17,18, and 24; one decimal place better on

equations 1, 2, 3, 5, 7, 8, 9, 10, 13, 15, 19, 20, 21, and 22; and two decimal places better on equations 4 and 23. The implicit method with  $p=4$  has been just better on equations 11, 12, 17 and 18; one decimal place better on equations 1, 2, 3, 4, 5, 6, 7, 8, 10, 13, 14, 15, 16, 19, 20, 21, 22, 23 and 24; and two decimal places better on equation 9.

The implicit method with  $p=5$  has been just better on equations 3, 10, 13, 15, 17 and 18; one decimal place better on equations 1, 4, 5, 6, 7, 8, 9, 14, 16, 19, 20, 21, 22, 23 and 24; and two decimal places better on equation 2.

The explicit method with  $p=4$ , however, has gone just worse for equations 11 and 12. The same has been observed in the case of implicit method with  $p=5$ .

## 2.5 Quadrature Optimal Multistep Methods in $H^2(c_r)$ Interpolatory for a set of Preassigned Functions

The coefficients  $\tilde{b}_j^F$  of a quadrature optimal multi-step formula, in  $H^2(c_r)$ ,

$$y_{n+1} - y_{n-s} = h \sum_{j=\delta_{to}}^m \tilde{b}_j^F f(x_{n+1-j}, y_{n+1-j}),$$

interpolatory for linearly independent functions  $\{\varphi_1, \dots, \varphi_p\}$  can be obtained by solving the system of linear equations

$$\begin{bmatrix} \tilde{C} & F^* \\ F & 0 \end{bmatrix} \begin{bmatrix} \tilde{b}^F \\ \lambda \end{bmatrix} = \begin{bmatrix} \tilde{d} \\ e \end{bmatrix}$$

where  $\tilde{C}$  and  $\tilde{d}$  are as in equation (9),  $\lambda = [\lambda_1, \dots, \lambda_p]^T$ ,  
 $\tilde{b}^F = [\tilde{b}_{\delta_{t_0}}^F, \dots, \tilde{b}_m^F]^T$ ,

$$F = [\varphi_i'(x_{n+1-j})]_{i=1, j=\delta_{t_0}}^{p, m},$$

$$e_i = \varphi_i(x_{n+1}) - \varphi_i(x_{n-s}), \quad i=1(1)p,$$

and 0 is  $p \times p$  null matrix.

Following theorem gives characterization of a quadrature optimal multistep method in  $H^2(c_r)$  interpolatory for a set of preassigned functions.

Theorem 4: A quadrature optimal multistep method in  $H^2(c_r)$  interpolatory for functions  $\{\varphi_1, \dots, \varphi_p\}$  is characterized by that it is locally interpolatory for constants and functions

$$\{\varphi_1, \dots, \varphi_p\} \cup \{h_k(x), k=p+\delta_{t_0}(1)m\}$$

where

$$\begin{aligned} h_k(x) = & \left\{ \frac{1}{\bar{x}_{n+1-k}} \log(r^{2-\bar{x}_{n+1-k}} x) \right\}^* \\ & + \sum_{j=\delta_{t_0}}^{p-1+\delta_{t_0}} \left\{ \sum_{q=\delta_{t_0}}^{p-1+\delta_{t_0}} \bar{w}_{j+1-\delta_{t_0}, q} \bar{\varphi}'_{q+1-\delta_{t_0}}(x_{n+1-k}) \right\} \\ & \cdot \left\{ \frac{1}{\bar{x}_{n+1-j}} \log(r^{2-\bar{x}_{n+1-j}} x) \right\}^* \end{aligned}$$

where

$$W = [w_{ij}]_{i=1(1)p, j=\delta_{t_0}(1)p-1+\delta_{t_0}}$$



with

$$W^{-1} = [\varphi_i^*(x_{n+1-j})]_{\substack{i=1(1)p \\ j=\delta_{t_0}(1)p-1+\delta_{t_0}}}$$

and  $\{.\}^*$  means the expression to be replaced by  $\frac{x}{r^2}$  if the denominator in the expression is zero.

Proof: The proof follows from Theorem 1.3 after a little simplification.

Table 2.7 corresponds to the quadrature optimal case interpolatory for functions  $\varphi_1(x) = \exp(1.6x)$  and  $\varphi_2(x) = \exp(-1.6x)$ . The behaviour of the error norms and the coefficients is found to be as in the case of quadrature optimal methods. The explicit method was found just better on equations 17,18 and 24; one decimal place better on equations 1,2,3,5,6,7,8,9,10,11,12,13,14,19,20 and 23; and two decimal places better on equations 4,15,16,21 and 22 as compared with the usual method. The implicit method has been just better on equations 17,18 and 24; one decimal place better on equations 1,4,5,6,7,11,12,13,14,15,16,19,22, 20,21,23; and two decimal places better on equations 2,3, 8,9, and 10.

## 2.6 Limiting Behaviour of the Coefficients as $r \rightarrow \infty$

From Tables 2.1-2.6 we observe that the coefficients of the quadrature optimal multistep formula/interpolatory for polynomials of a given degree are approximately the



same as the corresponding coefficients in the usual formula for the points under consideration near the centre of the circle  $c_r$  (or loosely speaking when the points are well inside the domain of the space). Properties of coefficients such as this have been considered in [7], [24], [30], [39] and [40]. For the space  $H^2(c_r)$ , Kaul [30] and Finney and Price Jr. [24] have studied the behaviour of coefficients in quadrature formulae as  $r \rightarrow \infty$ . The basic approach for such a study is given by Barnhill [7].

The following results give analogues of such behaviour of coefficients for quadrature multistep formulae in  $H^2(c_r)$  interpolatory for polynomials/arbitrary functions as  $r \rightarrow \infty$ . The basic tool in the analysis is provided by:

Theorem 5: Let

$$(16) \quad Y_{n+1} = Y_{n-s} + h \sum_{j=\delta_{to}}^m b_j^F f(x_{n+1-j}, Y_{n+1-j})$$

be a quadrature type multistep formula interpolatory for  $\{\varphi_{\delta_{to}}, \dots, \varphi_m\}$  and let the matrix  $[\varphi_i'(x_{n+1-j})]_{i,j=\delta_{to}}^m$  be non-singular. Let

$$(17) \quad Y_{n+1} = Y_{n-s} + h \sum_{j=\delta_{to}}^m b_{jr}^F f(x_{n+1-j}, Y_{n+1-j})$$

be a quadrature optimal multistep formula in  $H^2(c_r)$

interpolatory for  $\{\varphi_{\delta_{t0}}, \dots, \varphi_{p-1+\delta_{t0}}\}$ ,  $0 \leq p \leq m-\delta_{t0}$ ,  
 ( $p=0$  implies non-interpolatory case for these functions).

If the quadrature error functional  $\tilde{Q}_{nr}^F$  for (17) satisfies

$$(18) \quad \lim_{r \rightarrow \infty} \tilde{Q}_{nr}^F(\varphi_j^i) = 0, \quad j = p + \delta_{t0}(1)m,$$

then

$$\lim_{r \rightarrow \infty} \tilde{b}_{jr}^F = b_j^F, \quad j = \delta_{t0}(1)m.$$

Proof: Let

$$G = [\varphi_i^i(x_{n+1-j})]_{i,j=\delta_{t0}}^m,$$

$$B^F = [b_{\delta_{t0}}^F, \dots, b_m^F]^T,$$

$$\tilde{B}_r^F = [\tilde{b}_{\delta_{t0}r}^F, \dots, \tilde{b}_{mr}^F]^T,$$

and

$$Q_r = [\tilde{Q}_{nr}^F(\varphi_{\delta_{t0}}^i), \dots, \tilde{Q}_{nr}^F(\varphi_m^i)].$$

Since (16) is exact for the functions  $\varphi_{\delta_{t0}}, \dots, \varphi_m$  and

(17) is exact for  $\varphi_{\delta_{t0}}, \dots, \varphi_{p-1+\delta_{t0}}$ , writing the

formulae (16) and (17) for the functions  $\varphi_{\delta_{t0}}, \dots, \varphi_m$

and subtracting we get

$$hGB_r^F + Q_{nr} - hGB^F = 0.$$

In view of (18) and the interpolatory nature of (17) for

the functions  $\varphi_i$ ,  $i = \delta_{t0}(1)p + \delta_{t0} - 1$ ,  $Q_r \rightarrow 0$  as

$r \rightarrow \infty$ . Hence

$$\lim_{r \rightarrow \infty} hG(\tilde{B}_r^F - B^F) = 0$$

Since the matrix  $G$  is non-singular we have

$$\lim_{r \rightarrow \infty} \tilde{B}_r^F = B^F,$$

which proves the result.

Theorem 6. In  $H^2(c_r)$  the coefficients  $\tilde{b}_{jr}$  of a quadrature optimal multistep formula

$$(19) \quad Y_{n+1} = Y_{n-s} + h \sum_{j=\delta_{t0}}^m \tilde{b}_{jr} f(x_{n+1-j}, Y_{n+1-j})$$

approach the coefficients of the corresponding usual formula as  $r \rightarrow \infty$ .

Proof: Let  $Q_n$  denote the quadrature error functional of a usual formula

$$(20) \quad Y_{n+1} = Y_{n-s} + \sum_{j=\delta_{t0}}^m b_j f(x_{n+1-j}, Y_{n+1-j}).$$

Then

$$Q_n(x^i) = 0, \quad 0 \leq i \leq m - \delta_{t0}.$$

In view of Theorem 5 we need to prove that the quadrature error  $\tilde{Q}_n$  in (19) satisfies

$$\lim_{r \rightarrow \infty} \tilde{Q}_n(x^i) = 0, \quad 0 \leq i \leq m - \delta_{t0}.$$

Since (19) is quadrature optimal,  $\|\tilde{Q}_n\| \leq \|Q_n\|$ . Hence as  $\{\Psi_k\}_{k=0}^{\infty}$  as defined in (3) is a complete orthonormal sequence in  $H^2(c_r)$ , we have, equivalently,

$$\sum_{i=0}^{\infty} |\tilde{Q}_n(\Psi_i)|^2 \leq \sum_{k=0}^{\infty} |Q_n(\Psi_k)|^2,$$

giving

$$\sum_{i=0}^{\infty} r^{-2i} |\tilde{Q}_n(x^i)|^2 \leq \sum_{k=m+1-\delta_{t_0}}^{\infty} r^{-2k} |Q_n(x^k)|^2.$$

Taking a fixed  $i$ ,  $0 \leq i \leq m - \delta_{t_0}$  we get

$$|\tilde{Q}_n(x^i)|^2 \leq \sum_{k=m+1-\delta_{t_0}}^{\infty} r^{-2(k-i)} |Q_n(x^k)|^2, \text{ in which}$$

the expression on the right side approaches zero as  $r \rightarrow \infty$ , completing the proof.

Theorem 7: In  $H^2(c_r)$ , the coefficients  $\tilde{b}_{jr}^P$  of a quadrature optimal multistep formula

$$(21) \quad Y_{n+1} = Y_{n-s} + h \sum_{j=\delta_{t_0}}^m \tilde{b}_{jr}^P f(x_{n+1-j}, Y_{n+1-j}),$$

interpolatory for polynomials of degree  $p < m+1-\delta_{t_0}$ , approach the coefficients of the corresponding usual formula as  $r \rightarrow \infty$ .

Proof: The quadrature error functional  $\tilde{Q}_n^P$  for (21) satisfies

$$(22) \quad \tilde{Q}_n^P(x^i) = 0, \quad 0 \leq i \leq p-1$$

Proceeding as in the proof of Theorem 6,  $\|\tilde{Q}_n^P\| \leq \|Q_n\|$  gives

$$\sum_{i=p}^{\infty} r^{-2i} |\tilde{Q}_n^P(x^i)|^2 \leq \sum_{k=m+1-\delta_{t_0}}^{\infty} r^{-2k} |Q_n(x^k)|^2.$$

For any value of  $i$ ,  $p \leq i \leq m - \delta_{t0}$  we have, therefore,

$$|\tilde{Q}_n^p(x^i)|^2 \leq \sum_{k=m+1-\delta_{t0}}^{\infty} r^{-2(k-1)} |Q_n(x^k)|^2.$$

Thus

$$(23) \quad \lim_{r \rightarrow \infty} \tilde{Q}_n^p(x^i) = 0, \quad p \leq i \leq m - \delta_{t0}.$$

Using Theorem 5, (22) and (23) we get the result.

Theorem 8: If the  $(m + \delta_{t1}) \times (m + \delta_{t1})$  matrix

$$M = \begin{bmatrix} \varphi_1^i(x_{n+1-\delta_{t1}}) & \dots & \varphi_1^i(x_{n+1-m}) \\ \vdots & & \vdots \\ \varphi_p^i(x_{n+\delta_{t1}}) & \dots & \varphi_p^i(x_{n+1-m}) \\ 1 & \dots & 1 \\ x_{n+\delta_{t1}} & \dots & x_{n+1-m} \\ \vdots & & \vdots \\ x_{n+\delta_{t1}}^{m-p-\delta_{t0}} & \dots & x_{n+1-m}^{m-p-\delta_{t0}} \end{bmatrix}$$

is non-singular, in  $H^2(c_r)$  the coefficients  $\tilde{b}_{jr}^F$  of a quadrature optimal multistep formula

$$(24) \quad Y_{n+1} = Y_{n-s} + h \sum_{j=\delta_{t0}}^m \tilde{b}_{jr}^F f(x_{n+1-j}, Y_{n+1-j}),$$

interpolatory for functions  $\{\varphi_1, \dots, \varphi_p\}$  approach the coefficients  $b_j^F$  of the unique multistep formula

$$(25) \quad Y_{n+1} = Y_{n-s} + h \sum_{j=\delta_{t0}}^m b_j^F f(x_{n+1-j}, Y_{n+1-j})$$

interpolatory for  $\{\varphi_1, \dots, \varphi_p, x, x^2, \dots, x^{m-p+\delta_{t1}}\}$ .

Proof: The condition that the matrix  $M$  is non-singular is sufficient for the formula (25) to be unique. As both the formulae (24) and (25) are interpolatory for  $\{\varphi_1, \dots, \varphi_p\}$ , in view of Theorem 5 we need to prove that

$$\lim_{r \rightarrow \infty} \tilde{Q}_n^F(x^i) = 0, \quad i=0, \dots, m-p-1+\delta_{t1},$$

where  $\tilde{Q}_n^F$  denotes the quadrature error functional for (24). Proceeding as in Theorem 6 we get

$$|\tilde{Q}_n^F(x^i)|^2 \leq \sum_{k=m-p+\delta_{t1}}^{\infty} r^{-2(k-i)} |Q_n^F(x^k)|, \quad 0 \leq i \leq m-p-1+\delta_{t1}$$

where  $Q_n^F$  is the quadrature error functional for the method (25). Hence

$$\lim_{r \rightarrow \infty} |\tilde{Q}_n^F(x^i)|^2 = 0, \quad 0 \leq i \leq m-p+\delta_{t0},$$

completing the proof.

## 2.7 A Comparison of Different Methods

In Table 2.8 we present the end point ( $x_N=1.2$ ) errors for the set of twenty four differential equations for  $m=1(1)4$  step methods of usual and quadrature optimal type in  $H^2(c_r)$ . Even one step explicit and implicit methods have given better results for equations 1-23. In equation 24 however, the method has gone worse than the usual method. In fact for this equation one step usual method has worked better than the other methods of the usual type. The 4 step quadrature optimal methods have

Table 2.8

SITUATION:  $Y'$  IN  $H^2(C, r)$ ;  $R = 2.01$   $H = .10$   
 ERRORS AT END POINT FOR EXPLICIT METHODS

Eq.No.	M	1		2		3		4	
		USUAL	OPTIMAL	USUAL	OPTIMAL	USUAL	OPTIMAL	USUAL	OPTIMAL
1.		-0.41E-01	-0.36E-01	0.25E-02	0.74E-03	-0.30E-02	-0.11E-02	0.12E-03	0.12E-03
2.		-0.63E-01	-0.46E-01	0.14E-02	0.33E-03	-0.17E-02	-0.62E-03	0.15E-03	0.15E-03
3.		-0.39E-01	-0.35E-01	0.24E-02	0.66E-03	-0.54E-02	-0.20E-02	0.32E-03	0.32E-03
4.		-0.12E-00	-0.11E-00	0.40E-02	0.22E-02	-0.90E-02	-0.36E-02	0.53E-03	0.53E-03
5.		-0.44E-01	-0.40E-01	0.59E-02	0.22E-02	-0.69E-02	-0.22E-02	0.53E-03	0.53E-03
6.		-0.56E-01	-0.46E-01	0.96E-02	0.42E-02	-0.11E-01	-0.34E-02	0.89E-03	0.89E-03
7.		-0.81E-01	-0.73E-01	0.84E-02	0.26E-02	-0.94E-01	-0.37E-02	0.59E-03	0.59E-03
8.		-0.20E-01	-0.18E-01	0.34E-02	0.14E-02	-0.37E-01	-0.10E-01	0.20E-03	0.20E-03
9.		-0.11E-01	-0.16E-01	0.17E-02	0.66E-03	-0.21E-01	-0.75E-02	0.61E-03	0.61E-03
10.		-0.13E-01	-0.11E-01	0.76E-03	0.27E-03	-0.29E-01	-0.93E-02	0.99E-03	0.99E-03
11.		-0.13E-01	-0.11E-01	0.76E-03	0.27E-03	-0.29E-01	-0.93E-02	0.99E-03	0.99E-03
12.		-0.99E-02	-0.85E-02	0.18E-03	0.98E-04	-0.17E-01	-0.79E-02	0.50E-03	0.50E-03
13.		-0.85E-02	-0.70E-02	0.20E-03	0.68E-04	-0.20E-01	-0.65E-02	0.50E-03	0.50E-03
14.		-0.80E-02	-0.70E-02	0.20E-03	0.68E-04	-0.20E-01	-0.65E-02	0.50E-03	0.50E-03
15.		-0.69E-02	-0.60E-02	0.16E-03	0.29E-04	-0.15E-01	-0.61E-02	0.43E-03	0.43E-03
16.		-0.67E-02	-0.61E-02	0.82E-06	0.22E-05	-0.13E-01	-0.61E-02	0.43E-03	0.43E-03
17.		-0.66E-02	-0.60E-02	0.79E-05	0.21E-05	-0.13E-01	-0.61E-02	0.43E-03	0.43E-03
18.		-0.63E-02	-0.48E-02	0.53E-03	0.79E-04	-0.71E-01	-0.33E-02	0.60E-03	0.60E-03
19.		-0.60E-02	-0.48E-02	0.53E-03	0.79E-04	-0.71E-01	-0.33E-02	0.60E-03	0.60E-03
20.		-0.55E-02	-0.48E-02	0.53E-03	0.79E-04	-0.71E-01	-0.33E-02	0.60E-03	0.60E-03
21.		-0.52E-02	-0.48E-02	0.53E-03	0.79E-04	-0.71E-01	-0.33E-02	0.60E-03	0.60E-03
22.		-0.47E-02	-0.48E-02	0.53E-03	0.79E-04	-0.71E-01	-0.33E-02	0.60E-03	0.60E-03
23.		-0.46E-02	-0.48E-02	0.53E-03	0.79E-04	-0.71E-01	-0.33E-02	0.60E-03	0.60E-03
24.		-0.46E-02	-0.48E-02	0.53E-03	0.79E-04	-0.71E-01	-0.33E-02	0.60E-03	0.60E-03

ERRORS AT END POINT FOR IMPLICIT METHODS

Eq.No.	M	1		2		3		4	
		USUAL	OPTIMAL	USUAL	OPTIMAL	USUAL	OPTIMAL	USUAL	OPTIMAL
1.		-0.19E-03	-0.82E-04	0.27E-03	0.17E-03	-0.58E-04	-0.61E-05	0.63E-04	0.63E-05
2.		-0.12E-03	-0.44E-04	0.16E-03	0.69E-04	-0.28E-04	-0.15E-05	0.27E-04	0.27E-05
3.		-0.31E-03	-0.16E-03	0.47E-03	0.21E-03	-0.12E-03	-0.15E-04	0.14E-03	0.14E-04
4.		-0.20E-03	-0.94E-04	0.30E-03	0.11E-03	-0.62E-04	-0.57E-05	0.60E-04	0.60E-05
5.		-0.36E-03	-0.11E-03	0.47E-03	0.21E-03	-0.80E-04	-0.44E-05	0.80E-04	0.80E-05
6.		-0.45E-03	-0.23E-04	0.58E-04	0.22E-04	-0.17E-04	-0.25E-05	0.21E-04	0.21E-05
7.		-0.79E-04	-0.45E-05	0.94E-05	0.33E-05	-0.28E-05	-0.42E-06	0.32E-05	0.32E-06
8.		-0.68E-04	-0.31E-04	0.84E-04	0.28E-04	-0.19E-04	-0.25E-05	0.21E-04	0.21E-05
9.		-0.28E-04	-0.15E-04	0.33E-04	0.11E-04	-0.76E-05	-0.98E-06	0.80E-05	0.80E-06
10.		-0.11E-01	-0.54E-02	0.21E-01	0.88E-02	-0.25E-02	-0.33E-04	0.20E-02	0.20E-03
11.		-0.18E-01	-0.83E-02	0.28E-01	0.88E-02	-0.30E-02	-0.33E-04	0.20E-02	0.20E-03
12.		-0.18E-01	-0.83E-02	0.28E-01	0.88E-02	-0.30E-02	-0.33E-04	0.20E-02	0.20E-03
13.		-0.15E-01	-0.15E-05	0.14E-04	0.72E-05	-0.10E-04	-0.20E-06	0.49E-06	0.49E-06
14.		-0.12E-01	-0.21E-05	0.14E-04	0.72E-05	-0.10E-04	-0.20E-06	0.49E-06	0.49E-06
15.		-0.16E-01	-0.11E-05	0.20E-04	0.69E-05	-0.14E-04	-0.15E-06	0.68E-06	0.68E-06
16.		-0.13E-01	-0.25E-06	0.16E-04	0.11E-07	-0.11E-04	-0.08E-06	0.68E-06	0.68E-06
17.		-0.73E-07	-0.32E-07	0.76E-07	0.00E-07	-0.46E-08	-0.08E-08	0.00E-08	0.00E-08
18.		-0.71E-06	-0.30E-06	0.73E-06	0.00E-06	-0.22E-07	-0.22E-07	0.00E-07	0.00E-07
19.		-0.28E-03	-0.33E-04	0.66E-03	0.00E-03	-0.33E-03	-0.00E-03	0.00E-03	0.00E-03
20.		-0.63E-04	-0.74E-05	0.41E-04	0.19E-04	-0.33E-04	-0.00E-04	0.00E-04	0.00E-04
21.		-0.28E-03	-0.10E-04	0.57E-03	0.00E-03	-0.33E-03	-0.00E-03	0.00E-03	0.00E-03
22.		-0.17E-03	-0.23E-04	0.32E-03	0.00E-03	-0.33E-03	-0.00E-03	0.00E-03	0.00E-03
23.		-0.32E-03	-0.14E-03	0.34E-03	0.00E-03	-0.33E-03	-0.00E-03	0.00E-03	0.00E-03
24.		0.46E-06	0.17E-04	-0.11E-04	-0.19E-04	0.16E-05	0.16E-05	0.17E-04	0.20E-04

shown better performance over the usual ones in all cases. The performance of the quadrature optimal methods over the corresponding usual methods increased gradually with step  $m=1(1)4$ . This is as one might expect from Figure 2.1 and Figure 2.2 where we have plotted the norm of local truncation errors. In Figure 2.1,  $\log_{10}(\|\tilde{T}_n\|)$  and  $\log_{10}(\|T_n\|)$  have been plotted for the explicit case, and the same is done in Figure 2.2 for implicit case. It is interesting to note that the norms of local truncation errors for quadrature optimal methods are all through less than those of the usual methods.

In Table 2.9 we present end point ( $x_N=1.2$ ) errors for the set of the twenty four differential equations obtained by applying the methods: explicit usual, quadrature optimal, quadrature optimal interpolatory for polynomial of degree  $p = 1(1)4$  and quadrature optimal interpolatory for the functions  $e^{\alpha x}$  with  $\alpha = \pm 1.6$ . In Table 2.10 the same information has been given for implicit methods.

It follows from the Tables 2.9 and 2.10 that the quadrature optimal ones have remained the best among the usual, quadrature optimal, quadrature optimal interpolatory for polynomials ( $\tilde{M}^p$ ,  $p=1,2,\dots$ ) and interpolatory for functions  $\exp(1.6x)$  and  $\exp(-1.6x)$  (denoted as  $\tilde{M}^F$ )-methods except in a few cases (e.g. the explicit method interpolatory



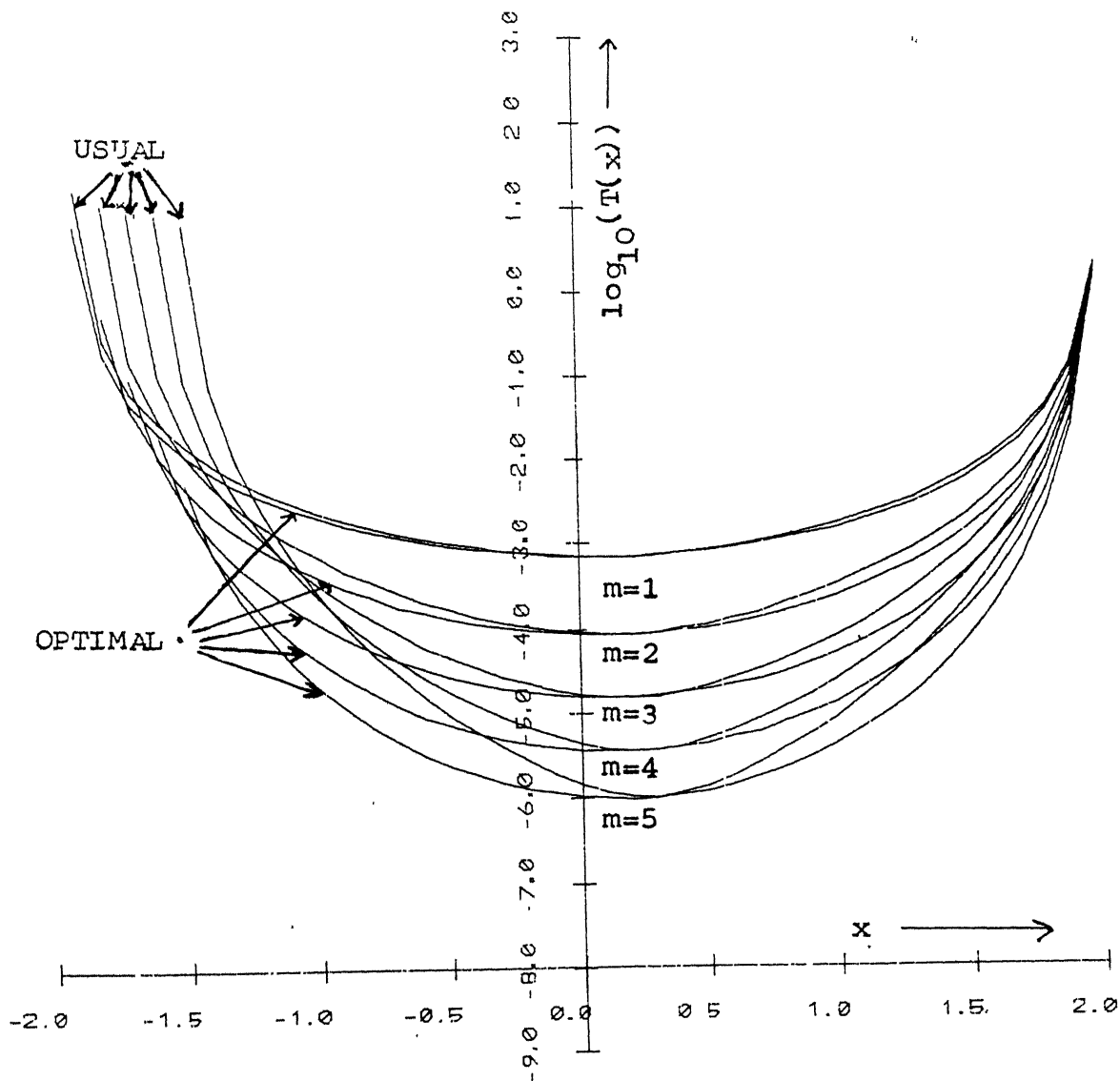


Figure 2.1: Local Truncation Error in Explicit  $H^2(c_r)$ -Quadrature Optimal Multistep Methods/Usual Methods ( $r=2.01$ ,  $h=0.1$ )

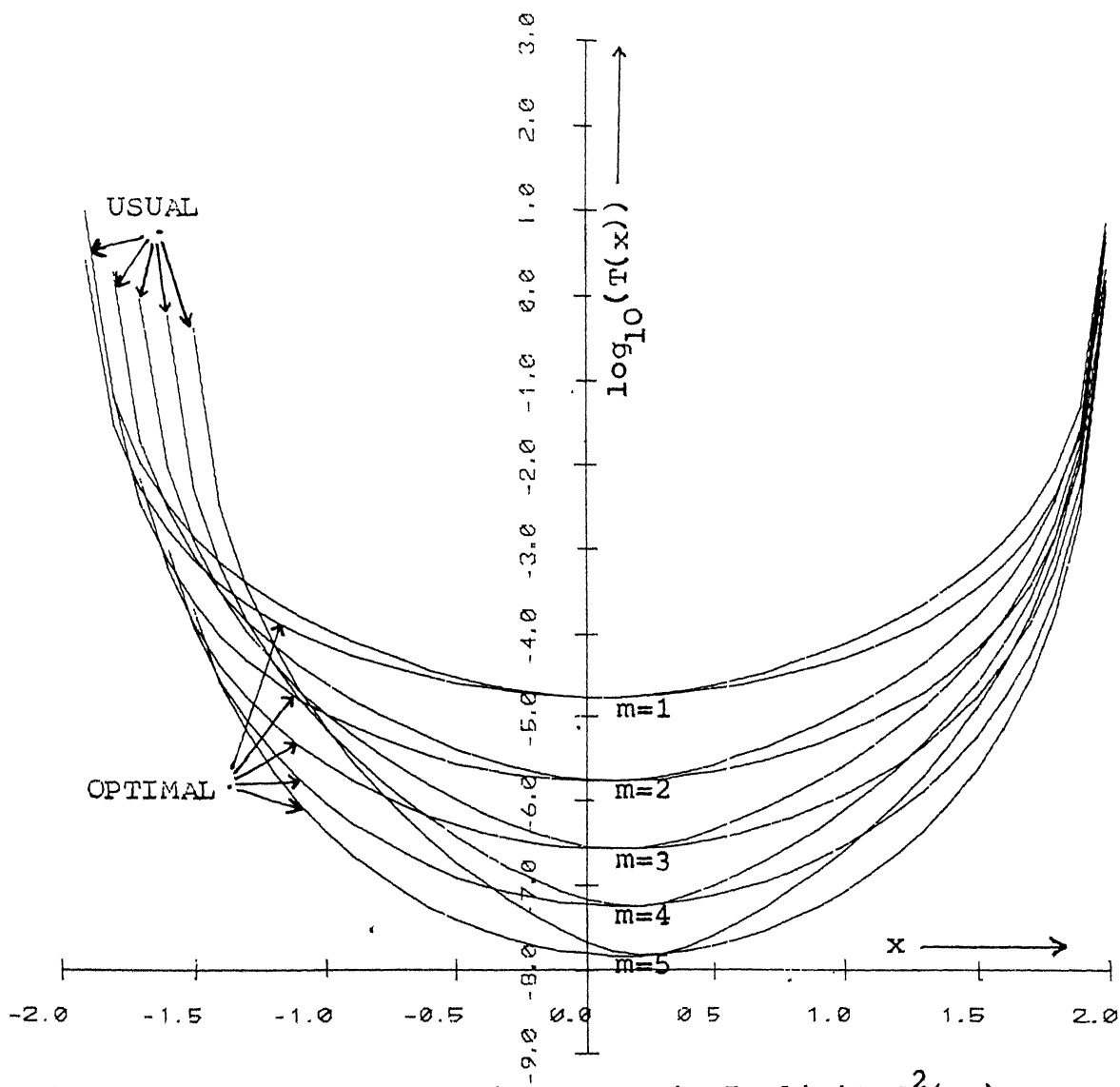


Figure 2.2: Local Truncation Error in Implicit  $H^2(c_r)$ -  
 Quadrature Optimal Multistep Methods/Usual  
 Methods ( $r=2.01$ ,  $h=0.1$ )

End point ( $x_N=1, 2$ ) errors for explicit  $H^2(c_r)$  quadrature  
optimal multistep methods

## Methods

Eqn. No.	Usual	$\tilde{M}$	$M^1$	Methods	$M^2$	$M^3$	$M^4$	$M^F$
1	-.27E-02	-.13E-03	-.13E-03	-.13E-03	-.13E-03	-.22E-03	-.33E-03	-.18E-03
2	-.93E-03	-.43E-04	-.43E-04	-.38E-04	-.38E-04	-.73E-04	-.32E-04	-.50E-04
3	-.61E-03	-.29E-03	-.30E-03	-.33E-03	-.33E-03	-.52E-03	-.91E-03	-.45E-03
4	-.24E-02	-.11E-03	-.11E-03	-.11E-03	-.11E-03	-.18E-03	-.21E-03	-.15E-03
5	.30E-02	.16E-03	.16E-03	.13E-03	.13E-03	.26E-03	.21E-03	.17E-03
6	-.97E-03	-.44E-04	-.44E-04	-.50E-04	-.50E-04	-.84E-04	.16E-03	.11E-05
7	-.16E-03	-.69E-05	-.70E-05	-.82E-05	-.82E-05	.14E-04	.26E-04	.12E-04
8	.92E-03	-.37E-04	-.38E-04	-.41E-04	-.41E-04	.75E-04	.11E-03	.61E-04
9	-.37E-03	-.14E-04	-.14E-04	-.17E-04	-.17E-04	.30E-04	.44E-04	.25E-04
10	-.48E-01	-.35E-02	-.35E-02	-.34E-02	-.34E-02	.47E-02	.73E-02	.41E-02
11	-.33E+02	-.13E+01	-.13E+01	-.16E+01	-.16E+01	.18E+02	.34E+02	-.89E+01
12	.33E+02	.89E+00	-.96E+00	.13E+01	.13E+01	.17E+02	.34E+02	.88E+01
13	-.16E-04	-.41E-05	-.42E-05	-.66E-06	-.66E-06	.63E-05	.63E-05	.75E-06
14	-.10E-04	-.35E-05	-.35E-05	-.42E-06	-.42E-06	.50E-05	.46E-05	.10E-05
15	-.22E-04	-.36E-05	-.37E-05	-.12E-05	-.12E-05	.66E-05	.76E-05	.60E-06
16	-.15E-04	-.30E-05	-.30E-05	-.80E-06	-.80E-06	.53E-05	.58E-05	.18E-06
17	-.70E-07	-.32E-08	-.33E-08	-.64E-08	-.64E-08	.26E-07	.38E-07	.15E-07
18	-.52E-06	-.30E-07	-.30E-07	-.61E-07	-.61E-07	.26E-06	.35E-06	.15E-06
19	-.70E-02	-.23E-03	-.22E-03	-.23E-03	-.23E-03	.66E-03	.16E-02	.56E-03
20	-.14E-02	-.18E-04	-.17E-04	.17E-04	.17E-04	.78E-04	.22E-03	.72E-04
21	-.10E-02	-.56E-05	-.38E-05	.28E-05	.28E-05	.61E-04	.14E-03	.51E-04
22	.24E-02	-.56E-04	-.51E-04	.53E-04	.53E-04	.23E-03	.44E-03	.18E-03
23	.27E-02	-.61E-05	.27E-03	.22E-03	.22E-03	.16E-03	.66E-04	.76E-04
24	-.71E-04	.19E-04	.21E-04	.24E-04	.24E-04	.12E-04	.17E-04	.78E-05

End point ( $x_N = 1.2$ ) errors for implicit  $H^2(c_r)$  quadrature optimal  
multistep methods

( $r=2.01$ ,  $h=0.1$ )

Eqn. No.	Usual	$\tilde{M}$	$\tilde{M}^1$	$\tilde{M}^2$	$\tilde{M}^3$	$\tilde{M}^4$	$\tilde{M}^5$	$\tilde{M}^F$
1	-.82E-04	-.15E-05	-.15E-05	-.17E-05	-.21E-05	-.51E-05	-.83E-05	-.24E-05
2	-.24E-04	-.11E-06	-.11E-06	-.24E-06	-.12E-06	-.12E-05	.11E-06	-.37E-06
3	-.19E-03	-.40E-05	-.41E-05	-.45E-05	-.59E-05	-.13E-04	-.24E-04	-.63E-05
4	-.69E-04	-.75E-06	.76E-06	-.91E-06	-.10E-05	-.33E-05	-.32E-05	-.13E-05
5	.86E-04	.83E-06	.83E-06	.14E-05	.12E-05	.52E-05	.41E-05	.21E-05
6	-.32E-04	-.79E-06	-.79E-06	-.87E-06	-.11E-05	.22E-05	.46E-05	-.11E-05
7	-.53E-05	-.12E-06	-.12E-06	-.13E-06	-.17E-06	-.36E-06	-.77E-06	-.17E-06
8	-.29E-04	-.60E-06	-.60E-06	-.67E-06	-.76E-06	-.18E-05	-.29E-05	-.82E-06
9	-.12E-04	-.18E-06	-.18E-06	-.19E-06	-.25E-06	-.70E-06	-.12E-05	-.26E-06
10	-.67E-03	.44E-05	.44E-05	.23E-05	.10E-04	-.96E-04	.29E-03	.60E-07
11	-.39E+00	.38E-01	.38E-01	.36E-01	-.15E+00	-.47E+00	.54E+00	.66E-01
12	.39E+00	-.26E-01	-.27E-01	-.26E-01	.14E+00	.48E+00	-.54E+00	-.61E-01
13	-.18E-06	.30E-07	.41E-07	.75E-08	.56E-07	-.67E-07	.12E-07	-.26E-07
14	-.12E-06	.34E-07	.34E-07	.00E+00	.45E-07	-.48E-07	.71E-06	-.19E-07
15	-.28E-06	.30E-07	.32E-07	.56E-08	.50E-07	-.84E-07	.16E-06	-.17E-07
16	-.18E-06	.26E-07	.24E-07	.19E-08	.43E-07	-.65E-07	.11E-06	-.13E-07
17	-.84E-09	.16E-09	.16E-09	.19E-09	.33E-09	.44E-09	.47E-09	.29E-09
18	-.51E-08	.23E-08	.23E-08	.23E-08	.42E-08	-.37E-08	.37E-08	.28E-08
19	-.22E-03	-.12E-04	-.12E-04	-.13E-04	-.14E-04	-.20E-04	-.32E-04	-.15E-04
20	-.46E-04	.17E-05	.18E-05	-.20E-05	-.25E-05	-.40E-05	-.68E-05	-.29E-05
21	-.32E-04	.17E-05	.18E-05	-.19E-05	-.19E-05	-.28E-05	-.71E-05	-.23E-05
22	-.72E-04	-.48E-05	-.49E-05	-.51E-05	-.48E-05	-.62E-05	-.71E-05	-.52E-05
23	.77E-04	-.61E-05	-.61E-05	-.51E-05	-.34E-05	.24E-05	.22E-05	-.25E-05
24	-.21E-05	-.44E-05	-.46E-06	-.55E-06	-.61E-06	-.68E-06	-.58E-06	-.84E-06

for 2 degree polynomials has performed better than optimal for equations 13,14,15 and 16; the explicit method interpolatory for  $\exp(1.6x)$  and  $\exp(-1.6x)$  has performed better on equations 13, 14, 15 and 16; the implicit method interpolatory for 2 degree polynomials has performed better on equations 13, 14, 15 and 16 and interpolatory for  $\exp(1.6x)$  and  $\exp(-1.6x)$  has performed better for equation 10).

## CHAPTER 3

### OPTIMAL MULTISTEP METHODS IN $H^2(c_r)$

#### 3.1 Introduction

Quadrature optimal multistep methods in  $H^2(c_r)$  described in Chapter 2 have been seen to be locally interpolatory for functions  $\log(r^2 - \bar{x}_{n+1-i}x)$ . In this chapter we study the corresponding optimal multistep methods in the space  $H^2(c_r)$ . As will be seen these optimal formulae are locally interpolatory for the functions  $x(r^2 - \bar{x}_{n+1-i}x)^{-2}$  the growth of which in the peripheral region of  $D_r$  is of a higher order than that of the corresponding functions in the quadrature optimal case.

Thus as compared to the quadrature optimal formulae of Chapter 2, the formulae obtained in this chapter will be better suited for differential equations whose solutions have more pronounced singularities outside  $c_r$ .

In Section 3.2 we give a direct proof that the derivative of the kernel function of  $H^2(c_r)$  is the complex conjugate of the representer of the derivative evaluation functional in  $H^2(c_r)$ . In Section 3.3 we describe the equations pertaining to optimal multistep methods in  $H^2(c_r)$  and their numerical implementation. Numerical results are presented for the set of differential

equations described at the end of Chapter 1. In Section 3.4 optimal methods interpolatory for polynomials of certain degree are described. In Section 3.5 we consider optimal methods interpolatory for a fixed set of functions. In Section 3.6 we establish the limiting behaviour of the coefficients as  $r \rightarrow \infty$ . In Section 3.7 a comparison of different methods is given.

### 3.2 The Representer of Derivative Evaluation Functional

In Chapter 2 we established that the derivative evaluation functional at any point inside the disk  $D_r = \{z: |z| < r\}$  is a bounded functional in  $H^2(c_r)$ . As  $H^2(c_r)$  possesses a reproducing kernel function

$$(1) \quad K(z, \bar{t}) = \frac{r}{2\pi(r^2 - z\bar{t})} ,$$

the representer  $D(t, \bar{z}_0)$  of the derivative evaluation functional at a point  $z_0 \in D_r$  ought to satisfy

$$\begin{aligned} D(t, \bar{z}_0) &= \overline{\frac{\partial}{\partial z} K(z, \bar{t})} \Big|_{z=z_0} \\ &= \frac{rt}{2\pi(r^2 - \bar{z}_0 t)^2} . \end{aligned}$$

This has been used in Chapter 2, while calculating the expression for the local truncation error. For the space  $H^2(c_r)$ , we directly verify, in the following theorem, that  $D(t, \bar{z}_0)$  as given above is indeed the representer of the derivative evaluation functional.

Theorem 1: The function

$$(2) \quad D(t, \bar{z}_0) = \frac{rt}{2\pi(r^2 - \bar{z}_0 t)^2} \in H^2(C_r)$$

is the representer of derivative evaluation functional at  $z_0 \in D_r$ .

Proof: The only singularity of  $D(t, \bar{z}_0)$  is a pole of order two at  $t = r^2/\bar{z}_0$ , which lies outside  $C_r$ . Hence the function belongs to  $H^2(C_r)$ . To complete the proof we need to show that

$$f'(z_0) = (f(t), \frac{rt}{2\pi(r^2 - \bar{z}_0 t)^2}).$$

By a Cauchy integral formula

$$\begin{aligned} f'(z_0) &= \frac{1}{2\pi i} \int_{C_r} \frac{f(t)}{(t-z_0)^2} dt \\ &= \frac{1}{2\pi i} \int_0^{2\pi} \frac{f(t)}{(re^{i\theta} - z_0)^2} re^{i\theta} i d\theta \\ &= \frac{r}{2\pi} \int_0^{2\pi} \frac{f(t) r^2 e^{-i\theta}}{(r^2 - rz_0 e^{-i\theta})^2} d\theta \\ &= \frac{r}{2\pi} \int_{C_r} \frac{f(t) \bar{t}}{(r^2 - z_0 \bar{t})^2} ds \\ &= (f(t), \frac{rt}{2\pi(r^2 - \bar{z}_0 t)^2}), \end{aligned}$$

which proves the result.



### 3.3 Optimal Multistep Methods in $H^2(c_r)$

For determining the coefficients  $\hat{b}_j$  of an optimal multistep formula

$$(3) \quad Y_{n+1} = \sum_{i=1}^m a_i Y_{n+1-i} + h \sum_{j=\delta_{to}}^m \hat{b}_j f(x_{n+1-j}, Y_{n+1-j}),$$

where  $a_i$ 's are prefixed according to some consistent and stable known usual formula, we have the normal equations

$$(4) \quad \hat{C} \hat{b} = \hat{d}$$

with  $\hat{b} = [\hat{b}_{\delta_{to}}, \dots, \hat{b}_m]^T$ ,

$$(5) \quad \hat{c}_{ij} = \frac{r(r^2 + x_{n+1-j} \bar{x}_{n+1-i})}{2\pi(r^2 - x_{n+1-j} \bar{x}_{n+1-i})^3}$$

and

$$(6) \quad \hat{d}_i = \frac{r}{2\pi h} \left[ \bar{x}_{n+1-i} \left\{ \frac{1}{(r^2 - x_{n+1} \bar{x}_{n+1-i})^2} - \sum_{k=1}^m \frac{a_k}{(r^2 - x_{n+1-k} \bar{x}_{n+1-i})^2} \right\} \right],$$

$$i, j = \delta_{to}(1)m,$$

which may be solved by Gaussian elimination after cancelling the common factor  $r/2\pi$  in  $\hat{c}_{ij}$  and  $\hat{d}_i$ . Moreover, removing  $h$  from  $\hat{d}_i$  results in  $h\hat{b}$  instead of  $\hat{b}$ .

The following theorem characterizes the optimal multistep formula (3) in  $H^2(c_r)$ .

Theorem 2. The optimal multistep formula (3) in  $H^2(c_r)$ , in which  $a_i$ 's are prefixed, is characterized by that it is locally interpolatory for functions

$$y_i(x) = \frac{x}{(r^2 - \bar{x}_{n+1-i}x)^2}, \quad i = \delta_{to}(1)m.$$

Proof: The proof immediately follows from Theorem 1.4 using (1) and (2).

Corollary 1. If  $x_{n+1-i} = 0$  for some  $i = \delta_{to}(1)m$  in (3), the formula (3) becomes consistent.

Proof: Since the corresponding usual formula is consistent, by its precision for constants,  $\sum a_i = 1$ . Further, by Theorem 2, if  $x_{n+1-i} = 0$ , (3) is exact for  $y(x) = x$ . These two facts combined make (3) consistent.

Analogues of Corollary 1 in the case of quadrature formulae have been considered in [30] and [39-40].

The  $H^2(c_r)$  norm of the local truncation error  $T_n$  for a general multistep formula

$$y_{n+1} = \sum_{i=1}^m a_i y_{n+1-i} + h \sum_{j=\delta_{to}}^m b_j f(x_{n+1-j}, y_{n+1-j})$$

is easily seen to be given by

$$\begin{aligned}
(7) \quad ||T_n||^2 &= \frac{r}{2\pi} \left[ \frac{1}{r^2 - |x_{n+1}|^2} - \sum_{i=1}^m a_i \frac{1}{r^2 - \bar{x}_{n+1} x_{n+1-i}} \right. \\
&\quad - \sum_{i=1}^m \bar{a}_i \left\{ \frac{1}{r^2 - x_{n+1} \bar{x}_{n+1-i}} - \sum_{j=1}^m a_j \frac{1}{r^2 - x_{n+1-j} \bar{x}_{n+1-i}} \right\} \\
&\quad - h \sum_{j=\delta_{to}}^m b_j g(x_{n+1-j}) \\
&\quad \left. - h \sum_{k=\delta_{to}}^m \bar{b}_k \{ g(x_{n+1-k}) - h \sum_{j=\delta_{to}}^m b_j \frac{r^2 + x_{n+1-j} \bar{x}_{n+1-k}}{(r^2 - x_{n+1-j} \bar{x}_{n+1-k})^3} \} \right]
\end{aligned}$$

where

$$g(x) = x \left[ \frac{1}{(r^2 - \bar{x}_{n+1} x)^2} - \sum_{l=1}^m \bar{a}_l \frac{1}{(r^2 - \bar{x}_{n+1-l} x)^2} \right].$$

In view of Theorem 2, or equivalently the normal equations (4), the norm of  $\hat{T}_n$ , the local truncation error for optimal formula (3), simplifies to

$$\begin{aligned}
(8) \quad ||\hat{T}_n||^2 &= \frac{r}{2\pi} \left[ \frac{1}{r^2 - |x_{n+1}|^2} - \sum_{i=1}^m a_i \frac{1}{r^2 - \bar{x}_{n+1} x_{n+1-i}} \right. \\
&\quad - \sum_{i=1}^m \bar{a}_i \left\{ \frac{1}{r^2 - x_{n+1} \bar{x}_{n+1-i}} - \sum_{j=1}^m a_j \frac{1}{r^2 - x_{n+1-j} \bar{x}_{n+1-i}} \right\} \\
&\quad \left. - h \sum_{j=\delta_{to}}^n \hat{b}_j g(x_{n+1-j}) \right].
\end{aligned}$$

In Table 3.1 we present the norm of local truncation errors and the coefficients of implicit and

explicit 5-step optimal multistep methods in  $H^2(c_r)$ , where the corresponding usual methods are the Adams-Moulton and the Adams-Bashforth. The coefficients have the same general behaviour as in the case of quadrature optimal methods (i.e., all the coefficients vary from point to point and that, excepting the first coefficient of the implicit method, all the other coefficients have increasing magnitude).

The local truncation error norm at the beginning i.e. at  $x = -1.5$  has reduced (as compared to  $\tilde{M}$  case) and now it is approximately  $1/7000$  of the local truncation error norm for usual method. The general behaviour of  $||\hat{T}_n||$  is observed to be as in the case of the quadrature optimal methods  $\tilde{M}$  of Chapter 2.

In Tables 3.1(a)-3.1(d) we present numerical results obtained by using the coefficients given in Table 3.1 on the set of twenty four differential equations. We observe that the explicit method is just better on differential equations 16 and 24 ; one decimal place better on equations 2,8,10,11,12,15,17,18,19,20 and 23; and two decimal places better on equations 1,3,4,5,6,7,9,21 and 22, as compared with the corresponding usual method. The implicit method is just better on equations 15,16 and 17; one decimal place better on equations 5, 12,18,19,20,21,22,23 and 24; two decimal places better on equations 2,3,4,6,7,8,10 and 11; and three decimal places better on equations 1 and 9.













As compared with the results of Chapter 2, we observe that when the singularities of the solutions are near  $c_r$ , the optimal methods have performed better and in the situations where the singularities were comparatively far from  $c_r$ , the quadrature optimal methods have worked better. (e.g. for equations 1,2,3,4,5,6,7,8 and 9 the optimal method is better than the quadrature optimal method while for equations 13,14,15 and 16 the quadrature optimal method has worked better.)

### 3.4 Optimal Multistep Methods in $H^2(c_r)$ Interpolatory for polynomials

In Section 1.6 we have described optimal multistep methods interpolatory for polynomials of certain degree. In this section we describe a  $H^2(c_r)$  situation taking the points  $x_{n+1-i}$  on a straight line in the domain of  $H^2(c_r)$ . We assume that the points are equispaced and separated by a distance  $h$ .

Reasoning as in Section 2.4 to get an optimal multistep formula we have to determine the optimal coefficients  $\hat{\gamma}_j^p$  in the formula interpolatory polynomials of degree  $p$  given by

$$\begin{aligned}
 (9) \quad Y_{n+1} - \sum_{i=1}^m a_i Y_{n+1-i} - h \sum_{j=0}^{p-1} \gamma_j^u \nabla^j f(x_{n+\delta_{t1}}, Y_{n+\delta_{t1}}) \\
 = h \sum_{j=p}^{m-\delta_{t0}} \hat{\gamma}_j^p \nabla^j f(x_{n+\delta_{t1}}, Y_{n+\delta_{t1}})
 \end{aligned}$$

where with prefixed  $a_i$ 's,  $\gamma_j^u$ 's are as in the corresponding usual formula. The normal equations are easily seen to be

$$(10) \quad \hat{C}^p \hat{\gamma}^p = \hat{d}^p$$

where

$$\hat{\gamma}^p = (\hat{\gamma}_p, \dots, \hat{\gamma}_{m-\delta_{t0}})^T,$$

$$\hat{C}_{ij}^p = \frac{r}{2\pi} \sum_{k=0}^j \sum_{l=0}^i (-1)^{l+k} \binom{i}{l} \binom{j}{k} \frac{r^{2+x_{n+\delta_{t1}-k}} \bar{x}_{n+\delta_{t1}-l}}{(r^{2-x_{n+\delta_{t1}-k}} \bar{x}_{n+\delta_{t1}-l})^3},$$

and

$$\begin{aligned} \hat{d}_i^p = & \frac{r}{2\pi h} \left[ \sum_{l=0}^i (-1)^l \binom{i}{l} \left\{ \frac{\bar{x}_{n+\delta_{t1}-l}}{(r^{2-x_{n+1}} \bar{x}_{n+\delta_{t1}-l})^2} \right. \right. \\ & \left. \left. - \sum_{q=1}^m \frac{a_q \bar{x}_{n+\delta_{t1}-l}}{(r^{2-x_{n+1}-q} \bar{x}_{n+\delta_{t1}-l})^2} \right\} \right] \\ & - \frac{r}{2\pi} \sum_{q=0}^{p-1} \gamma_q^u \left\{ \sum_{k=0}^q \sum_{l=0}^i (-1)^{l+k} \binom{i}{l} \binom{q}{k} \right. \\ & \left. \frac{r^{2+x_{n+\delta_{t1}-k}} \bar{x}_{n+\delta_{t1}-l}}{(r^{2-x_{n+\delta_{t1}-k}} \bar{x}_{n+\delta_{t1}-l})^3} \right\}, \\ & i, j = p(1)m-\delta_{t0}. \end{aligned}$$

In view of Theorem 1.6 we have:

**Theorem 3:** The optimal multistep formula (9) is characterized by that it is locally interpolatory for functions  $\{x^i, i=1(1)p\} \cup \{h_j(x); j=p(1)m-\delta_{t0}\}$ , where

$$h_j(x) = \sum_{k=0}^j (-1)^k \binom{j}{k} \frac{x}{(r^2 - \bar{x}_{n,\delta} t_1^{-k} x)^2}.$$

In Tables 3.2 to 3.6 we present the coefficients  $\hat{b}_j^p$  (calculated via  $\hat{\gamma}_j^p$ ) and error norms for  $H^2(c_r)$ -optimal 5-step methods interpolatory for polynomials of degree  $p$ ,  $1 \leq p \leq 5$ . The general behaviour of the error norms and the coefficients has been same as in the case of the quadrature optimal multistep methods interpolatory for certain degree polynomials. A summary of the numerical results obtained by applying these coefficients on the twenty four differential equations is as follows:

As compared with the usual explicit case, the  $H^2(c_r)$  explicit optimal 5-step method with  $p=1$  has performed just better on equation 24; one decimal place better on equations 2, 5, 10, 11, 12, 18, 19, 22 and 23; two decimal places better on equations 1, 3, 4, 6, 7, 8, 20, 21 and 22; and two to three places better on equation 9. Similarly, as compared with the usual implicit 5-step method the implicit optimal 5-step method has performed just better on equations 15, 23 and 24; one decimal place better on equations 3, 5, 12, 18, 19, 20, 21 and 22; two decimal places better on equation 9. In the case of equations 13, 14, 15, 16 and 17, however, the performance of both the usual and the optimal methods has been comparable.

SITUATION: Y IN H<sup>+</sup>(C F)  
MULTI STEP METHOD OF 5 STEPS

Table 3.3

SITUATION: Y IN  $(C, r)$  R = 2.01 Hz  $\cdot 10^{10}$   
MULTI STEP METHOD OF 5 STEPS INTERPOLATRY UPTO 2 DEGREE POLYNOMIALS

[illegible]

Table 3.4

[illegible]









The explicit method with  $p=2$  has performed just better on equations 15, 23 and 24; one decimal place better on equations 2, 13, 15, 19, 22 and 23; and two decimal places better on equations 1, 3, 4, 5, 6, 7, 8, 9, 10, 20 and 21. The implicit method has performed just better on equations 11, 12, 14 and 24; one decimal place better on equations 13, 15, 16, 17, 18, 19, 20, 21, 22, and 23; two decimal places better on equations 1, 2, 3, 4, 5, 6, 7, 8 and 10; and three decimal places better on equation 9.

The explicit method with  $p=3$  has worked just better on equation 24; one decimal place better on equations 1, 2, 5, 6, 8, 9, 10, 15, 16, 19, 20, 22 and 23; and two decimal places better on equations 3 and 4. The implicit method has worked just better on equations 5 and 24; one decimal place better on equations 5, 10, 16, 19, 20, 21, 22 and 23; two decimal places better on equations 1, 2, 3, 4, 6 and 7; and three decimal places better on equations 8 and 9. The usual and optimal methods on equations 11, 12, 13, 14, 17 and 18 have performed almost comparably. .

The explicit method with  $p=4$  has worked just better on equations 10, 13, 14, 15 and 24; one decimal place better on equations 2, 5, 6, 8, 19, 20, 22 and 23; and two decimal places better on equations 1, 3, 4, 7, 9 and 21. The implicit method has been just better on equations 10, 13, 14, 15 and 24; one decimal place better on equations 1, 3, 4, 5, 6, 7, 8, 19, 20, 2, 2;

22 and 23; and two decimal places better on equation 9. On equations 11 and 12 the performance of usual and optimal methods has been almost similar.

The implicit optimal method with  $p=5$  has been just better on equations 10, 13, 14, 15, 16, 17 and 18; one decimal place better on equations 1, 2, 3, 4, 5, 7, 19, 20, 21, 22, 23 and 24; two decimal places better on equations 6, 8 and 9. The optimal and usual methods have worked almost similarly on equations 11 and 12.

### 3.5 Optimal Multistep Methods in $H^2(c_r)$ Interpolatory for a Set of Preassigned Functions

The coefficients  $\hat{b}_j^F$  of an optimal multistep formula

$$(11) \quad y_{n+1} = \sum_{i=1}^m a_i y_{n+1-i} + h \sum_{j=\delta_{to}}^m \hat{b}_j^F f(x_{n+1-j}, y_{n+1-j})$$

in  $H^2(c_r)$  with prefixed  $a_i$ 's interpolatory for linearly independent functions  $\{\varphi_1, \dots, \varphi_p\}$  are to satisfy the normal equations

$$(12) \quad \begin{bmatrix} \hat{C} & F^* \\ F & 0 \end{bmatrix} \begin{bmatrix} \hat{b}^F \\ \lambda \end{bmatrix} = \begin{bmatrix} \hat{d} \\ e \end{bmatrix}$$

with  $\hat{C}, \hat{d}$  as in equations (4),  $\lambda = [\lambda_1, \dots, \lambda_p]^T$ ,  $\hat{b}^F = [\hat{b}_{\delta_{to}}^F, \dots, \hat{b}_m^F]^T$ ,

$$(13) \quad F = [\varphi_i'(x_{n+1-j})]_{i=1, j=\delta_{to}}^{p,m},$$

$$(14) \quad e_i = \varphi_i(x_{n+1}) - \sum_{j=1}^m a_j \varphi_i(x_{n+1-j}), \quad i=1(1)p$$

and  $0$  is a  $p \times p$  null matrix.

This method is characterized as follows:

Theorem 4: An optimal multistep method in  $H_-^2(c_r)$  interpolatory for linearly independent functions  $\{\varphi_1, \dots, \varphi_p\}$  is characterized by that it is locally interpolatory for functions

$$\{\varphi_1, \dots, \varphi_p\} \cup \{h_k(x); k = \delta_{t0}(1)m-p\}$$

with

$$h_k(x) = \frac{x}{(r^2 - \bar{x}_{n+1-k}x)^2} + \sum_{i=m-p+1}^m \bar{g}_{i-m+p, k+1-\delta_{t0}} \frac{x}{(r^2 - \bar{x}_{n+1-i}x)^2}$$

$$\text{where } G = [g_{j,q}]_{\substack{j=1(1)p \\ q=1(1)m-p+\delta_{t1}}} \quad \text{with } G = W^{-1}E,$$

where

$$W = [\varphi_i^1(x_{n+1-j})]_{\substack{i=1(1)p \\ j=m+1-p(1)m}}$$

and

$$E = [\varphi_i^1(x_{n+1-j})]_{\substack{i=1(1)p \\ j=\delta_{t0}(1)m-p}}.$$

Proof: The proof follows from Theorem 18.

In Table 3.7 we have displayed the optimal case interpolatory for functions  $\varphi_1(x) = \exp(1.6x)$  and

SITUATION: Y IN H<sup>2</sup> C (C, T) R = 2.01 H = 1.0  
MULTI STEP METHOD OF 5 STEPS INTERPOLATORY FOR EXP(ALPHA\*X), ALPHA = 1.6 ALPHA = -1.6

X	EUSUAL	OPTIMAL	H X B(1)	H X B(2)	H X B(3)	H X B(4)	H X B(5)
1.50	0.690001	0.280002	0.175725	0.700000	0.450000	0.232001	0.172002
1.40	0.670002	0.590003	0.186712	0.500000	0.323000	0.406700	0.490000
1.30	0.900000	0.170003	0.198467	0.300000	0.802000	0.067000	0.847000
1.20	0.210004	0.680004	0.201960	0.200000	0.002000	0.918000	0.082000
1.10	0.260003	0.320004	0.213327	0.100000	0.144000	0.089000	0.408000
1.00	0.110004	0.180004	0.222888	0.200000	0.139000	0.080000	0.508000
0.90	0.550004	0.660005	0.236888	0.300000	0.181000	0.033000	0.945000
0.80	0.290004	0.450005	0.237356	0.400000	0.202000	0.028000	0.945000
0.70	0.160004	0.330005	0.237328	0.500000	0.220000	0.025000	0.945000
0.60	0.970005	0.250005	0.244621	0.600000	0.238000	0.022000	0.945000
0.50	0.610005	0.190005	0.246546	0.700000	0.254000	0.019000	0.945000
0.40	0.400005	0.160005	0.252211	0.800000	0.269000	0.016000	0.945000
0.30	0.270005	0.130005	0.255093	0.900000	0.283000	0.013000	0.945000
0.20	0.190005	0.110005	0.255093	1.000000	0.296000	0.010000	0.945000
0.10	0.120005	0.100005	0.255093	1.000000	0.309000	0.007000	0.945000
0.00	0.100005	0.100005	0.255093	1.000000	0.323000	0.004000	0.945000
0.10	0.120005	0.110005	0.255093	1.000000	0.336000	0.001000	0.945000
0.20	0.190005	0.130005	0.255093	1.000000	0.349000	0.000000	0.945000
0.30	0.270005	0.160005	0.255093	1.000000	0.362000	0.000000	0.945000
0.40	0.400005	0.190005	0.255093	1.000000	0.375000	0.000000	0.945000
0.50	0.610005	0.250005	0.255093	1.000000	0.388000	0.000000	0.945000
0.60	0.970005	0.330005	0.255093	1.000000	0.401000	0.000000	0.945000
0.70	1.600006	0.450005	0.255093	1.000000	0.414000	0.000000	0.945000
0.80	2.900006	0.660005	0.255093	1.000000	0.427000	0.000000	0.945000
0.90	5.500006	0.945005	0.255093	1.000000	0.440000	0.000000	0.945000
1.00	9.450006	0.945005	0.255093	1.000000	0.453000	0.000000	0.945000
1.10	16.000006	0.945005	0.255093	1.000000	0.466000	0.000000	0.945000
1.20	27.000006	0.945005	0.255093	1.000000	0.479000	0.000000	0.945000
1.30	40.000006	0.945005	0.255093	1.000000	0.492000	0.000000	0.945000
1.40	55.000006	0.945005	0.255093	1.000000	0.505000	0.000000	0.945000
1.50	72.000006	0.945005	0.255093	1.000000	0.518000	0.000000	0.945000
1.60	90.000006	0.945005	0.255093	1.000000	0.531000	0.000000	0.945000
1.70	109.000006	0.945005	0.255093	1.000000	0.544000	0.000000	0.945000
1.80	129.000006	0.945005	0.255093	1.000000	0.557000	0.000000	0.945000
1.90	150.000006	0.945005	0.255093	1.000000	0.570000	0.000000	0.945000
2.00	172.000006	0.945005	0.255093	1.000000	0.583000	0.000000	0.945000

X	EUSUAL	OPTIMAL	H X B(1)	H X B(2)	H X B(3)	H X B(4)	H X B(5)
1.50	0.320000	0.800000	0.417054	0.595000	1.055000	1.562000	2.100000
1.40	0.330000	0.810000	0.386666	0.930000	1.655000	2.100000	2.100000
1.30	0.340000	0.820000	0.355277	0.930000	2.255000	2.100000	2.100000
1.20	0.350000	0.830000	0.323889	0.930000	2.855000	2.100000	2.100000
1.10	0.360000	0.840000	0.292500	0.930000	3.455000	2.100000	2.100000
1.00	0.370000	0.850000	0.261111	0.930000	4.055000	2.100000	2.100000
0.90	0.380000	0.860000	0.229722	0.930000	4.655000	2.100000	2.100000
0.80	0.390000	0.870000	0.198333	0.930000	5.255000	2.100000	2.100000
0.70	0.400000	0.880000	0.166944	0.930000	5.855000	2.100000	2.100000
0.60	0.410000	0.890000	0.135556	0.930000	6.455000	2.100000	2.100000
0.50	0.420000	0.900000	0.104167	0.930000	7.055000	2.100000	2.100000
0.40	0.430000	0.910000	0.072778	0.930000	7.655000	2.100000	2.100000
0.30	0.440000	0.920000	0.041389	0.930000	8.255000	2.100000	2.100000
0.20	0.450000	0.930000	0.010000	0.930000	8.855000	2.100000	2.100000
0.10	0.460000	0.940000	0.000000	0.930000	9.455000	2.100000	2.100000
0.00	0.470000	0.950000	0.000000	0.930000	10.055000	2.100000	2.100000
0.10	0.480000	0.960000	0.000000	0.930000	10.655000	2.100000	2.100000
0.20	0.490000	0.970000	0.000000	0.930000	11.255000	2.100000	2.100000
0.30	0.500000	0.980000	0.000000	0.930000	11.855000	2.100000	2.100000
0.40	0.510000	0.990000	0.000000	0.930000	12.455000	2.100000	2.100000
0.50	0.520000	1.000000	0.000000	0.930000	13.055000	2.100000	2.100000
0.60	0.530000	1.010000	0.000000	0.930000	13.655000	2.100000	2.100000
0.70	0.540000	1.020000	0.000000	0.930000	14.255000	2.100000	2.100000
0.80	0.550000	1.030000	0.000000	0.930000	14.855000	2.100000	2.100000
0.90	0.560000	1.040000	0.000000	0.930000	15.455000	2.100000	2.100000
1.00	0.570000	1.050000	0.000000	0.930000	16.055000	2.100000	2.100000
1.10	0.580000	1.060000	0.000000	0.930000	16.655000	2.100000	2.100000
1.20	0.590000	1.070000	0.000000	0.930000	17.255000	2.100000	2.100000
1.30	0.600000	1.080000	0.000000	0.930000	17.855000	2.100000	2.100000
1.40	0.610000	1.090000	0.000000	0.930000	18.455000	2.100000	2.100000
1.50	0.620000	1.100000	0.000000	0.930000	19.055000	2.100000	2.100000
1.60	0.630000	1.110000	0.000000	0.930000	19.655000	2.100000	2.100000
1.70	0.640000	1.120000	0.000000	0.930000	20.255000	2.100000	2.100000
1.80	0.650000	1.130000	0.000000	0.930000	20.855000	2.100000	2.100000
1.90	0.660000	1.140000	0.000000	0.930000	21.455000	2.100000	2.100000
2.00	0.670000	1.150000	0.000000	0.930000	22.055000	2.100000	2.100000

$\varphi_2(x) = (-1.6x)$ . The behaviour of error norms and that of the coefficients is found to be as in other situations. The performance of the methods as compared to usual methods is as follows:

The explicit optimal method  $\hat{M}^F$  in  $H^2(c_r)$  has been just better on equations 14, 17, 18 and 24; one decimal place better on equations 2, 10, 11, 12, 13, 15, 16, 19, 20, 21, 22 and 23; and two decimal places better on equations 1, 3, 4, 5, 6, 7, 8 and 9. The implicit optimal method  $\hat{M}^F$  was observed just better on equations 14, 18, 23 and 24; one decimal place better on equations 12, 13, 15, 16, 17, 29, 20, 21 and 22; two decimal places better on equations 1, 3, 4, 5, 6, 7, 8, 10, and 11; and three decimal places better on equations 2 and 9.

### 3.6 Behaviour of the Coefficients as $r \rightarrow \infty$

In Section 2.6 we have studied the properties of the coefficients of quadrature optimal multistep methods in  $H^2(c_r)$ . Here we present the corresponding results for optimal multistep methods in  $H^2(c_r)$ . We first prove:

Theorem 5: Let

$$(15) \quad Y_{n+1} = \sum_{i=1}^m a_i Y_{n+1-i} + h \sum_{j=\delta_{to}}^m b_j^F f(x_{n+1-j}, Y_{n+1-j})$$

be a multistep formula interpolatory for functions  $\{\varphi_{\delta_{to}}, \dots, \varphi_m\}$  and let the matrix  $[\varphi_i'(x_{n+1-j})]_{i,j=\delta_{to}}^m$  be non-singular. Let

$$(16) \quad Y_{n+1} = \sum_{i=1}^m a_i Y_{n+1-i} + h \sum_{j=\delta_{to}}^m \hat{b}_{jr}^F f(x_{n+1-j}, Y_{n+1-j})$$

be an optimal multistep formula in  $H^2(c_r)$  interpolatory for  $\{\varphi_{\delta_{to}}, \dots, \varphi_{p-1+\delta_{to}}\}$ ,  $0 \leq p \leq m - \delta_{to}$  ( $p=0$  implies non-interpolatory case for these functions). If the local truncation error functional  $\hat{T}_{nr}^F$  for (16) satisfies

$$(17) \quad \lim_{r \rightarrow \infty} \hat{T}_{nr}^F(\varphi_j) = 0, \quad j = p + \delta_{to}(1)m$$

then

$$(18) \quad \lim_{r \rightarrow \infty} \hat{b}_{jr}^F = b_j^F, \quad j = \delta_{to}(1)m.$$

Proof: Let

$$G = [\varphi'(x_{n+1-j})]_{i,j=\delta_{to}}^m,$$

$$B^F = [b_{\delta_{to}}^F, \dots, b_m^F]^T,$$

$$\hat{B}_r^F = [\hat{b}_{\delta_{to}r}^F, \dots, \hat{b}_{mr}^F]^T,$$

and

$$\hat{T}_{nr} = [\hat{T}_{nr}^F(\varphi_{\delta_{to}}), \dots, \hat{T}_{nr}^F(\varphi_m)]^T.$$

Then, substituting the functions  $\varphi_{\delta_{to}}, \dots, \varphi_m$  in the formulae (15) and (16) and subtracting we get

$$hG \hat{B}_r^F + \hat{T}_{nr} - hGB^F = 0$$

Since  $\lim_{r \rightarrow \infty} \hat{T}_{nr} = 0$ , by (17), and as  $G$  is non-singular, the result is immediate.

Theorem 6: Let  $a_i, i=1(1)m$ , be constants such that  $\sum_{i=1}^m a_i = 1$ . Then the  $H^2(c_r)$ -coefficients  $\hat{b}_{jr}$  of an optimal multistep formula

$$(19) \quad Y_{n+1} = \sum_{i=1}^m a_i Y_{n+1-i} + h \sum_{j=\delta_{t0}}^m \hat{b}_{jr} f(x_{n+1-j}, Y_{n+1-j})$$

approach the coefficients  $b_j$  of multistep formula

$$(20) \quad Y_{n+1} = \sum_{i=1}^m a_i Y_{n+1-i} + h \sum_{j=\delta_{t0}}^m b_j f(x_{n+1-j}, Y_{n+1-j})$$

of maximal polynomial precision.

Proof: Since the formula (20) is interpolatory for polynomials of maximal degree and it is assumed that  $a_i$ 's are known constants with  $\sum a_i = 1$ , we know that the coefficients  $b_j$  of method (20) can uniquely be determined by using that it is interpolatory for functions  $\{x, x^2, \dots, x^{m+\delta_{t1}}\}$ . In view of Theorem 5 we need to prove that the truncation error functional  $\hat{T}_{nr}$  for (19) satisfies

$$\lim_{r \rightarrow \infty} \hat{T}_{nr}(x^i) = 0, \quad 0 \leq i \leq m + \delta_{t1}$$

The method (19) being optimal, we have

$$\|\hat{T}_{nr}\| \leq \|T_n\|$$

where  $T_n$  is the local truncation error functional for (20). Since  $\{\psi_k\}_{k=0}^{\infty}$ , as defined in (2.3), is a complete orthonormal sequence in  $H^2(c_r)$ , we have



$$\sum_{i=0}^{\infty} |\hat{T}_{nr}(\Psi_i)|^2 \leq \sum_{k=0}^{\infty} |T_n(\Psi_i)|^2 = \sum_{k=m+\delta_{t1}+1}^{\infty} \frac{1}{2\pi} r^{-2k-1} |T_n(x^k)|^2$$

Thus, for each fixed  $i$ ,  $0 \leq i \leq m + \delta_{t1}$ , we have

$$|\hat{T}_{nr}(x^i)|^2 \leq \sum_{k=m+\delta_{t1}+1}^{\infty} r^{-2(k-i)} |T_n(x^k)|^2$$

The expression on the right approaches 0 as  $r \rightarrow \infty$ . Hence

$$\lim_{r \rightarrow \infty} \hat{T}_{nr}(x^i) = 0, \quad 0 \leq i \leq m + \delta_{t1},$$

which proves the result.

Theorem 7. Let  $\sum_{i=1}^m a_i = 1$  where  $a_i$ 's are given constants.

The  $H^2(c_r)$ -coefficients  $\hat{b}_{jr}^p$  of an optimal multistep formula

$$(21) \quad y_{n+1} = \sum_{i=1}^m a_i y_{n+1-i} + h \sum_{j=\delta_{t0}}^m \hat{b}_{jr}^p f(x_{n+1-j}, y_{n+1-j}),$$

interpolatory for polynomials of degree  $p < m + \delta_{t1}$ ,

approach the coefficients of the corresponding usual formula as  $r \rightarrow \infty$ .

Proof: Since  $\sum_{i=1}^m a_i = 1$  the formula (21) is interpolatory for constants. As it is interpolatory for polynomials of degree  $p$ , the truncation error functional  $\hat{T}_{nr}^p$  of (21) satisfies

$$\hat{T}_{nr}^p(x^i) = 0, \quad 0 \leq i \leq p.$$

In view of Theorem 5 it suffices to prove that

$$\lim_{r \rightarrow \infty} \hat{T}_{nr}^P(x^i) = 0, \quad p+1 \leq i \leq m + \delta_{t1}$$

Since  $\|\hat{T}_{nr}^P\| \leq \|T_n\|$  where  $T_n$  denotes the truncation error functional of a usual method, as in Theorem 6, we have

$$\sum_{i=p+1}^{\infty} r^{-2i} |\hat{T}_{nr}^P(x^i)|^2 \leq \sum_{k=m+\delta_{t1}+1}^{\infty} r^{-2k} |T_n(x^k)|^2$$

Hence

$$|\hat{T}_{nr}^P(x^i)|^2 \leq \sum_{k=m+\delta_{t1}+1}^{\infty} r^{-2(k-i)} |T_n(x^k)|^2, \quad p+1 \leq i \leq m+\delta_{t1}$$

Since the right hand side approaches 0 as  $r \rightarrow \infty$  we have

$$\lim_{r \rightarrow \infty} \hat{T}_{nr}^P(x^i) = 0, \quad p+1 \leq i \leq m+\delta_{t1},$$

completing the proof.

Theorem 8: Let  $\sum_{i=1}^m a_i = 1$  where  $a_i$ 's are given constants.

Let the  $(m+\delta_{t1}) \times (m+\delta_{t1})$  matrix

$$M = \begin{bmatrix} \varphi_1'(x_{n+\delta_{t1}}) & \dots & \varphi_1'(x_{n+1-m}) \\ \vdots & & \\ \varphi_p'(x_{n+\delta_{t1}}) & \dots & \varphi_p'(x_{n+1-m}) \\ 1 & \dots & 1 \\ x_{n+\delta_{t1}} & \dots & x_{n+1-m} \\ \vdots & & \\ x_{n+\delta_{t1}}^{m-p-\delta_{t0}} & \dots & x_{n+1-m}^{m-p-\delta_{t0}} \end{bmatrix}$$

be non-singular. Then, the  $H^2(c_r)$ -coefficient  $\hat{b}_{jr}^F$  of an optimal multistep formula

$$(2.2) \quad Y_{n+1} = \sum_{i=1}^m a_i Y_{n+1-i} + h \sum_{j=\delta_{t0}}^m \hat{b}_{jr}^F f(x_{n+1-j}, Y_{n+1-j}),$$

interpolatory for functions  $\{\varphi_1, \dots, \varphi_p\}$ ,  $p < m + \delta_{t1}$  approach the coefficients  $b_j^F$  of the unique multistep formula

$$(23) \quad Y_{n+1} = \sum_{i=1}^m a_i Y_{n+1-i} + h \sum_{j=\delta_{t0}}^m b_j^F f(x_{n+1-j}, Y_{n+1-j}),$$

interpolatory for functions  $\{\varphi_1, \dots, \varphi_p, x, x^2, \dots, x^{m-p+\delta_{t1}}\}$ .

Proof: The condition that the matrix  $M$  is non-singular is sufficient for the formula (23) to be determined uniquely. Since both the formulae are interpolatory for functions  $\{\varphi_1, \dots, \varphi_p\}$ , in view of Theorem 5 we need to prove only that the local truncation error functional  $\hat{T}_{nr}^F$  for (22) satisfies

$$\lim_{r \rightarrow \infty} \hat{T}_{nr}^F(x^i) = 0, \quad 1 \leq i \leq m-p+\delta_{t1}.$$

A similar procedure as in Theorem 6 gives

$$|\hat{T}_{nr}^F(x^i)|^2 \leq \sum_{k=m-p+\delta_{t1}+1}^m r^{-2(k-i)} |T_n^F(x^k)|^2, \quad 1 \leq i \leq m-p+\delta_{t1}$$

The right side of the above inequality approaches zero as  $r \rightarrow \infty$ . Hence

$$\lim_{r \rightarrow \infty} \hat{T}_{nr}^F(x^i) = 0, \quad 1 \leq i \leq m-p+\delta_{t1}$$

which proves the result.

### 3.7 A Comparison of Optimal Methods in $H^2(c_r)$

In Table 3.8 we present the end point ( $x_N=1.2$ ) errors for the set of twenty four differential equations for 1 to 4 step explicit and implicit methods alongwith the 1 to 4 step usual methods. We observe that the performance of the optimal methods has been better all through except in the case of equation 24, which seems to be a chance.

In Figure 3.1 we have plotted  $\log_{10}(\|\hat{T}_n\|)$  and  $\log_{10}(\|T_n\|)$  at different points for explicit methods of step 1 to 5. We observe that the error norm for the optimal method, as expected, remains throughout less than that of the usual method. In Figure 3.2 these norms have been plotted for the implicit methods.

In Table 3.9 we present the end point errors ( $x_N=1.2$ ) for the twenty four differential equations for 5 step explicit  $H^2(c_r)$  optimal method/interpolatory for polynomials of degree 1-4 (as denoted by  $\hat{M}^1, \hat{M}^2, \dots$ , the superscript digit denoting the degree of the polynomials for which it is interpolatory)/and interpolatory for  $\exp(1.6x)$ ,  $\exp(-1.6x)$  (denoted as  $\hat{M}^F$ ).

We observe that  $\hat{M}^F$  has performed best in many cases (e.g. explicit method for equations 9,13,14,15,16, 19,18 and 23) and  $\hat{M}^2$  on other equations (e.g. for equations 2,3,4,5,6 and 7). Other optimal methods have also performed best on selected equations.

Table 3.8

SITUATION: Y IN  $H^2$  (C r) ; R= 2.01 H= .10  
 ERRORS AT END POINT FOR EXPLICIT METHODS

Eq.No.	M	1		2		3		4	
		USUAL	OPTIMAL	USUAL	OPTIMAL	USUAL	OPTIMAL	USUAL	OPTIMAL
1.	-0	0.41E-01	0.25E-01	0.25E-02	0.24E-04	0.30E-02	0.74E-03	0.17E-02	0.71E-05
2.	-0	0.41E-01	0.18E-01	0.16E-02	0.26E-04	0.11E-02	0.48E-03	0.13E-02	0.22E-05
3.	-0	0.41E-01	0.23E-01	0.43E-02	0.37E-04	0.55E-02	0.75E-03	0.39E-02	0.35E-04
4.	-0	0.41E-01	0.36E-01	0.46E-02	0.20E-03	0.50E-02	0.17E-03	0.00E-02	0.00E-04
5.	-0	0.41E-01	0.36E-01	0.57E-02	0.14E-03	0.69E-02	0.10E-03	0.00E-02	0.00E-04
6.	-0	0.41E-01	0.53E-01	0.96E-02	0.52E-03	0.11E-03	0.14E-03	0.00E-02	0.00E-04
7.	-0	0.41E-01	0.53E-01	0.84E-02	0.34E-03	0.37E-03	0.39E-03	0.00E-02	0.00E-04
8.	-0	0.41E-01	0.14E-02	0.34E-03	0.00E-00	0.22E-03	0.43E-03	0.00E-02	0.00E-04
9.	-0	0.41E-01	0.60E-03	0.17E-03	0.00E-00	0.30E-03	0.11E-03	0.00E-02	0.00E-04
10.	-0	0.41E-01	0.58E-03	0.76E-03	0.00E-00	0.20E-03	0.81E-03	0.00E-02	0.00E-04
11.	-0	0.41E-01	0.49E-02	0.18E-03	0.00E-00	0.17E-03	0.12E-03	0.00E-02	0.00E-04
12.	-0	0.41E-01	0.42E-02	0.14E-03	0.00E-00	0.30E-03	0.10E-03	0.00E-02	0.00E-04
13.	-0	0.41E-01	0.43E-02	0.20E-03	0.00E-00	0.22E-03	0.94E-03	0.00E-02	0.00E-04
14.	-0	0.41E-01	0.36E-02	0.16E-03	0.00E-00	0.11E-03	0.81E-03	0.00E-02	0.00E-04
15.	-0	0.41E-01	0.46E-02	0.82E-03	0.00E-00	0.11E-03	0.30E-03	0.00E-02	0.00E-04
16.	-0	0.41E-01	0.43E-02	0.53E-03	0.00E-00	0.69E-03	0.26E-03	0.00E-02	0.00E-04
17.	-0	0.41E-01	0.11E-01	0.34E-03	0.00E-00	0.71E-03	0.11E-03	0.00E-02	0.00E-04
18.	-0	0.41E-01	0.11E-01	0.34E-03	0.00E-00	0.63E-03	0.76E-03	0.00E-02	0.00E-04
19.	-0	0.41E-01	0.46E-02	0.22E-03	0.00E-00	0.37E-03	0.60E-03	0.00E-02	0.00E-04
20.	-0	0.41E-01	0.46E-02	0.36E-03	0.00E-00	0.37E-03	0.45E-03	0.00E-02	0.00E-04
21.	-0	0.41E-01	0.42E-02	0.65E-04	0.00E-00	0.77E-04	0.35E-04	0.00E-02	0.00E-04

ERRORS AT END POINT FOR IMPLICIT METHODS

Eq.No.	M	1		2		3		4	
		USUAL	OPTIMAL	USUAL	OPTIMAL	USUAL	OPTIMAL	USUAL	OPTIMAL
1.	-0	0.19E-03	0.29E-04	0.27E-03	0.85E-04	0.58E-04	0.22E-07	0.69E-04	0.42E-05
2.	-0	0.31E-03	0.12E-04	0.16E-03	0.56E-04	0.28E-04	0.23E-05	0.14E-04	0.74E-05
3.	-0	0.40E-03	0.22E-04	0.47E-03	0.14E-03	0.12E-03	0.28E-03	0.82E-04	0.30E-05
4.	-0	0.40E-03	0.22E-04	0.30E-03	0.87E-04	0.62E-04	0.51E-06	0.60E-04	0.38E-05
5.	-0	0.40E-03	0.22E-04	0.47E-03	0.20E-04	0.80E-04	0.55E-06	0.21E-04	0.55E-05
6.	-0	0.40E-03	0.22E-04	0.58E-03	0.11E-04	0.17E-04	0.64E-06	0.21E-04	0.00E-06
7.	-0	0.40E-03	0.22E-04	0.94E-03	0.14E-04	0.28E-04	0.46E-06	0.22E-04	0.00E-06
8.	-0	0.40E-03	0.22E-04	0.33E-03	0.00E-05	0.76E-04	0.80E-06	0.22E-04	0.33E-06
9.	-0	0.40E-03	0.22E-04	0.22E-03	0.55E-05	0.25E-04	0.80E-06	0.20E-04	0.00E-06
10.	-0	0.40E-03	0.22E-04	0.21E-03	0.11E-02	0.60E-04	0.40E-06	0.19E-04	0.00E-06
11.	-0	0.40E-03	0.22E-04	0.28E-03	0.11E-02	0.60E-04	0.40E-06	0.19E-04	0.00E-06
12.	-0	0.40E-03	0.22E-04	0.18E-03	0.14E-04	0.10E-05	0.60E-06	0.69E-06	0.00E-06
13.	-0	0.40E-03	0.22E-04	0.14E-03	0.14E-04	0.68E-06	0.60E-06	0.49E-06	0.00E-06
14.	-0	0.40E-03	0.22E-04	0.20E-03	0.14E-04	0.14E-05	0.47E-06	0.97E-06	0.00E-06
15.	-0	0.40E-03	0.22E-04	0.16E-03	0.16E-04	0.96E-06	0.42E-06	0.69E-06	0.00E-06
16.	-0	0.40E-03	0.22E-04	0.73E-03	0.71E-09	0.46E-08	0.16E-08	0.33E-08	0.00E-06
17.	-0	0.40E-03	0.22E-04	0.73E-03	0.14E-06	0.36E-07	0.17E-07	0.19E-07	0.00E-06
18.	-0	0.40E-03	0.22E-04	0.66E-03	0.54E-06	0.13E-03	0.41E-04	0.10E-03	0.00E-06
19.	-0	0.40E-03	0.22E-04	0.77E-03	0.77E-03	0.23E-04	0.11E-04	0.23E-04	0.00E-06
20.	-0	0.40E-03	0.22E-04	0.78E-03	0.96E-04	0.33E-04	0.94E-05	0.60E-04	0.00E-06
21.	-0	0.40E-03	0.22E-04	0.32E-03	0.32E-03	0.55E-04	0.16E-05	0.26E-04	0.00E-06
22.	-0	0.40E-03	0.22E-04	0.14E-03	0.14E-03	0.72E-05	0.76E-05	0.74E-05	0.00E-06
23.	-0	0.40E-03	0.22E-04	0.23E-03	0.23E-03	0.19E-05	0.69E-05	0.19E-05	0.00E-06

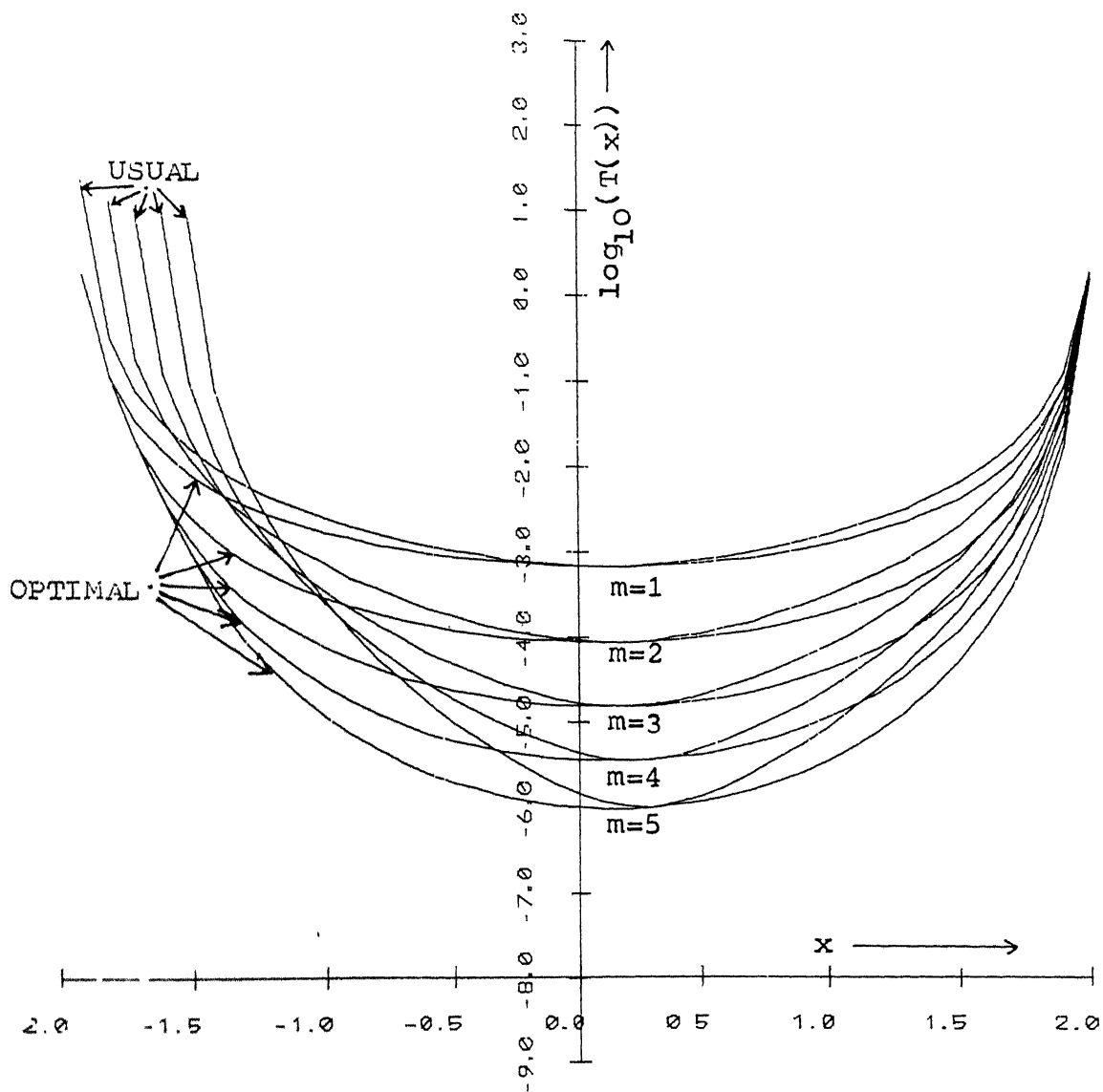


Figure 3.1: Local Truncation Error in Explicit  $H^2(c_r)$  -  
Optimal Multistep Methods/Usual Methods  
( $r=2.01$ ,  $h=0.1$ )

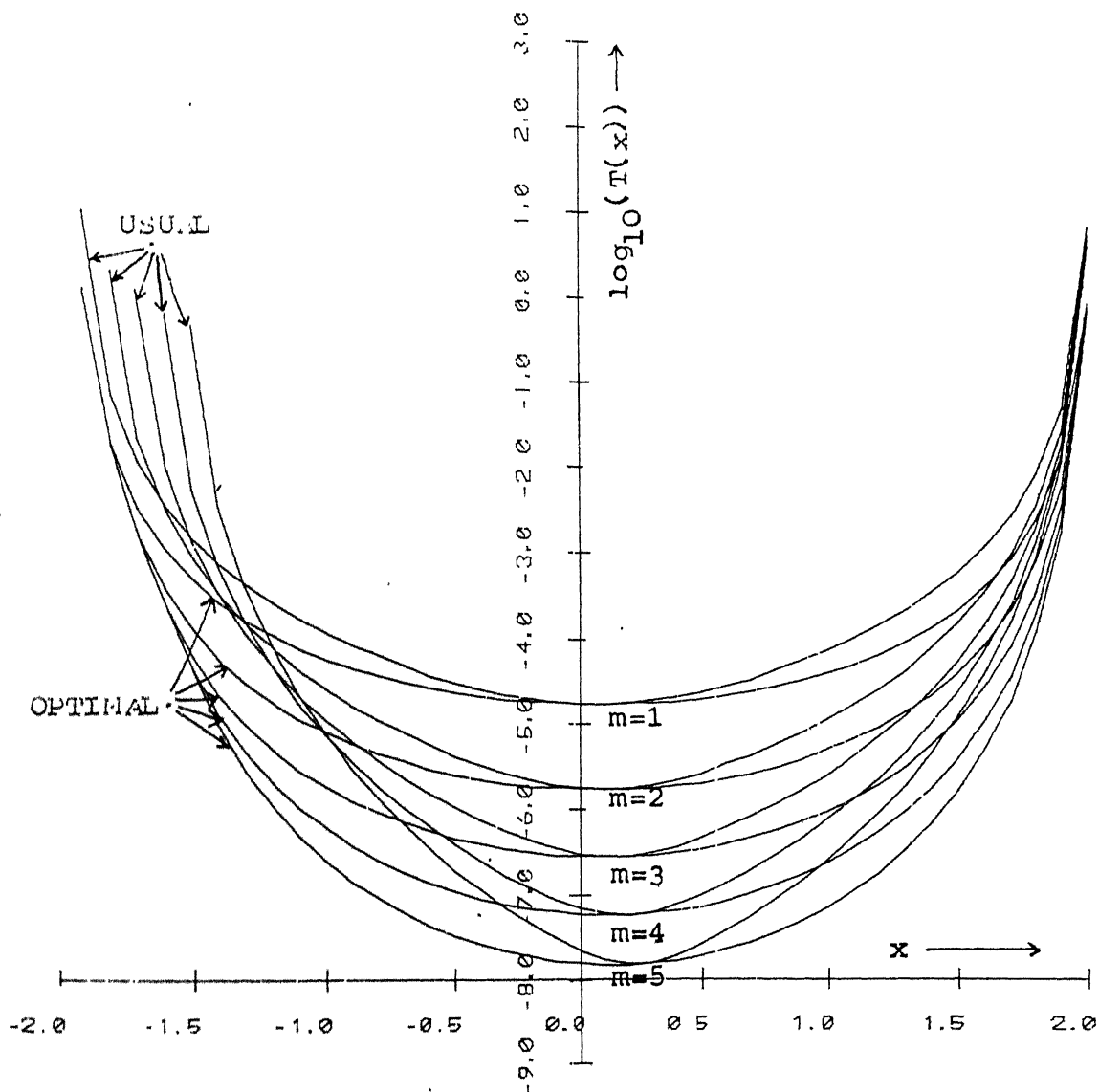


Figure 3.2: Local Truncation Error in Implicit  $H^2(c_r)$  -  
Optimal Multistep Methods/Usual Methods  
( $r=2.01$ ,  $h=0.1$ )

Table 3.9

End point ( $x_N=1.2$ ) errors for explicit  $H^2(c_r)$ -optimal methods  
( $r=2.01$ ,  $h=0.1$ )

Eqn. No.	Usual	Methods				
		$\hat{M}$	$\hat{M}^1$	$\hat{M}^2$	$\hat{M}^3$	$\hat{M}^4$
1	-.27E-02	-.71E-04	-.84E-04	-.31E-04	-.17E-03	-.29E-04
2	-.93E-03	-.40E-04	-.50E-04	.10E-05	-.86E-04	.11E-03
3	-.61E-03	-.13E-03	-.14E-03	-.10E-03	-.33E-03	-.13E-03
4	-.24E-02	-.63E-04	-.75E-04	-.23E-04	-.16E-03	.14E-03
5	.30E-02	.16E-03	.21E-03	-.73E-05	.28E-03	-.23E-03
6	-.97E-03	-.14E-04	-.15E-04	-.13E-04	-.50E-04	-.38E-04
7	-.16E-03	-.17E-05	-.18E-05	-.23E-05	-.83E-05	-.58E-05
8	.92E-03	-.14E-04	-.14E-05	-.39E-04	-.58E-04	.77E-05
9	-.37E-03	-.29E-05	-.26E-05	-.31E-05	-.23E-04	.50E-05
10	-.48E-01	-.27E-02	-.28E-02	-.15E-02	-.89E-02	.17E-01
11	-.33E+02	.19E+01	.21E+01	.14E+02	-.39E+02	.44E+02
12	.33E+02	-.26E+01	-.27E+01	-.14E+02	.39E+02	-.44E+02
13	-.16E-04	-.11E-04	-.16E-04	.46E-05	-.12E-04	.10E-04
14	-.10E-04	-.10E-04	-.15E-04	.40E-05	-.94E-05	.72E-05
15	-.22E-04	-.86E-05	-.12E-04	.39E-05	-.13E-04	.13E-04
16	-.15E-04	-.75E-05	-.11E-04	.35E-05	-.10E-04	.94E-05
17	-.70E-07	.63E-08	.85E-08	.11E-07	-.52E-07	.57E-07
18	-.52E-06	.68E-07	.92E-07	.12E-06	.51E-06	-.51E-06
19	-.70E-02	.13E-03	.31E-03	.43E-03	-.41E-03	-.91E-03
20	-.14E-02	.26E-04	.59E-04	.89E-04	-.96E-05	-.53E-04
21	-.10E-02	.23E-04	.62E-04	.92E-04	-.26E-04	-.82E-05
22	.24E-02	.55E-04	.15E-03	.20E-03	-.19E-03	-.19E-05
23	.27E-02	.41E-03	.70E-03	.34E-03	.18E-03	-.55E-03
24	-.71E-04	.23E-04	.45E-04	.60E-04	.27E-04	-.11E-04
						-.58E-04
						-.20E-04
						-.13E-03
						-.47E-04
						.87E-04
						-.17E-04
						-.24E-05
						-.10E-04
						-.35E-05
						-.21E-02
						.87E+01
						-.90E+01
						-.42E-05
						-.39E-05
						-.25E-05
						-.23E-05
						.12E-07
						.12E-06
						.12E-03
						.71E-04
						.78E-04
						.10E-03
						.43E-05
						.54E-04



End point ( $x_N=1.2$ ) errors for implicit  $H^2$ -( $c_F$ )-optimal methods

Eqn. No.	Usual
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Eqn. NO.	Usual	Methods						
		$\wedge_M$	$\wedge_M^1$	$\wedge_M^2$	$\wedge_M^3$	$\wedge_M^4$	$\wedge_M^5$	$\wedge_M^F$
1	-.82E-04	.10E-06	.22E-06	-.83E-06	.18E-06	-.40E-05	.14E-05	-.31E-06
2	-.24E-04	.36E-06	.48E-06	-.33E-06	.67E-06	-.16E-05	.33E-05	.13E-06
3	-.19E-03	-.51E-06	-.46E-06	-.16E-05	-.76E-06	-.83E-05	-.21E-05	-.12E-05
4	-.69E-04	.22E-06	.31E-06	-.51E-06	.69E-06	-.33E-05	.53E-05	-.52E-07
5	.86E-04	-.16E-05	-.21E-05	.15E-05	-.17E-05	.54E-05	-.66E-05	-.66E-06
6	-.32E-04	-.23E-06	-.25E-06	-.38E-06	-.26E-06	-.14E-05	-.10E-05	-.37E-06
7	-.53E-05	-.35E-07	-.37E-07	-.40E-07	-.19E-0	-.22E-06	-.17E-06	-.40E-07
8	-.29E-04	-.23E-06	-.26E-06	-.46E-06	.75E-08	-.14E-05	.45E-06	-.40E-06
9	-.12E-04	-.65E-07	-.67E-07	-.56E-07	.10E-06	-.51E-06	.15E-06	-.47E-07
10	-.67E-03	.10E-04	.12E-04	-.45E-05	.63E-04	-.20E-03	.42E-03	.75E-05
11	-.39E+00	-.98E-02	-.29E-02	-.11E+00	.61E+00	-.83E+00	.66E+00	-.25E-02
12	.39E+00	.36E-01	.27E-01	.12E+00	-.60E+00	.83E+00	-.66E+00	.13E-01
13	-.18E-06	.18E-06	.23E-06	-.10E-06	.15E-06	-.14E-06	.17E-06	.97E-07
14	-.12E-06	.16E-06	.22E-06	-.93E-07	.11E-06	-.10E-06	.10E-06	.97E-07
15	-.28E-06	.12E-06	.16E-06	-.78E-07	.15E-06	-.17E-06	.21E-06	.65E-07
16	-.18E-06	.10E-06	.14E-06	-.78E-07	.12E-06	-.12E-06	.15E-06	.12E-09
17	-.84E-09	-.12E-09	-.12E-09	.44E-10	.95E-09	-.73E-09	.64E-09	.63E-07
18	-.51E-08	0.0	0.0	.93E-09	.10E-07	-.61E-08	.51E-08	.23E-08
19	-.22E-03	-.42E-06	.42E-05	-.99E-05	-.10E-04	-.16E-04	-.73E-05	-.17E-04
20	-.46E-04	.13E-05	-.52E-06	-.68E-06	.12E-05	-.32E-05	-.18E-05	-.24E-05
21	-.32E-04	.10E-06	-.70E-06	-.17E-05	-.13E-05	-.27E-05	.22E-06	-.32E-05
22	-.72E-04	-.20E-05	-.38E-05	-.58E-05	-.39E-05	-.61E-05	.13E-05	-.86E-05
23	.77E-04	-.94E-05	-.14E-04	-.88E-05	-.82E-05	.18E-05	-.76E-05	-.18E-04
24	-.21E-05	.89E-06	.43E-06	-.16E-06	-.50E-06	-.76E-06	.42E-06	-.12E-05

In Table 3.10 we present the end point errors of 5-step implicit methods. Here we have a similar observation as in the case of explicit methods. Thus optimal methods interpolatory for polynomials/some other functions have performed better than optimal methods in selected situations.

## CHAPTER 4

### QUADRATURE OPTIMAL MULTISTEP METHODS IN $L^2(\hat{C}_r)$

#### 4.1 Introduction

The norm in the space  $H^2(c_r)$  is based on a line integral along the boundary  $c_r$  which takes care of the points in the interior of  $c_r$  only indirectly. Hence the points in the neighbourhood of the boundary receive a dominant weightage in the multistep methods corresponding to the space  $H^2(c_r)$ . As the maximum use of these methods is envisaged on a subinterval of  $(-r, r)$  it effectively means that the  $H^2(c_r)$  methods would, relatively, be more effective in the peripheral regions. On the contrary, in the case of the Hilbert space  $L^2(\hat{C}_r)$ , however, the norm corresponds to an area integral on the disk  $D_r$  and thus it intrinsically gives relatively more weightage to the points in the interior of  $c_r$ . The corresponding multistep methods are consequently expected to result in a better distributed behaviour in the central regions. It may also be noted that (as sets)  $L^2(\hat{C}_r) \supset H^2(c_r)$ .

This chapter is a study of quadrature optimal multistep methods in the space  $L^2(\hat{C}_r)$ . In Section 4.2 we define the space  $L^2(\hat{C}_r)$  and establish the boundedness of derivative evaluation functionals in  $L^2(\hat{C}_r)$ . In

Section 4.3 we present the quadrature optimal multistep methods in  $L^2(\hat{C}_r)$ . In Section 4.4 quadrature optimal multistep methods in  $L^2(\hat{C}_r)$ , interpolatory for polynomial of a particular degree, are presented. In Section 4.5 we describe quadrature optimal  $m$ -step methods interpolatory for arbitrary functions. In Section 4.6 we discuss the limiting behaviour of the coefficients and in Section 4.7 we present a comparison of various quadrature optimal multistep methods in  $L^2(\hat{C}_r)$ . To distinguish from the  $H^2(C_r)$  situation, in the notations we have used an under bar (e.g., as in  $\bar{b}_j$ ).

#### 4.2 The Space $L^2(\hat{C}_r)$ and Boundedness of Derivative Evaluations

Let  $L^2(D_r)$  denote the space of complex valued measurable functions  $h(x,y)$  defined on  $D_r = \{(x,y): x^2 + y^2 < r^2\}$  for which  $|h|$  is square integrable in  $D_r$ . The space  $L^2(D_r)$  turns out to be a complex Hilbert space, with the inner product

$$(h,k) = \iint_{D_r} h(x,y) \overline{k(x,y)} \, dx dy.$$

The subspace of  $L^2(D_r)$  consisting of functions of the type  $h(x,y) = f(z)$  ( $z = x+iy$ ), where  $f(z)$  is an analytic function of  $z$ , regular in  $D_r$ , is closed and has an infinite dimension. This is the Hilbert space  $L^2(\hat{C}_r)$  with the induced inner product given by

$$(1) \quad (f, g) = \int \int_{D_r} f(z) \overline{g(z)} \, dx dy .$$

The space  $L^2(\hat{c}_r)$  has a reproducing kernel function as

$$(2) \quad K(z, \bar{t}) = \frac{r^2}{\pi(r^2 - z\bar{t})^2}$$

and is separable with a complete orthonormal sequence  $\{\Psi_k\}$  of functions given by

$$(3) \quad \Psi_k(z) = \frac{z^k}{\sqrt{\pi} r^{k+1}}, \quad k = 0, 1, \dots$$

We prove that derivative evaluation of any order at a point inside  $c_r$  is a bounded functional:

Theorem 1: For  $z \in D_r$  and  $k$  any positive integer  $D_z^k$  is a bounded linear functional in  $L^2(\hat{c}_r)$  with

$$\|D^k(z)\| \leq k! \sqrt{\frac{r}{2\pi}} \left( \frac{2}{r-|z|} \right)^{k+\frac{3}{2}} .$$

Proof. By a cauchy integral formula we have

$$f^{(k)}(z) = \frac{k!}{2\pi i} \int_{c_\rho} \frac{f(\omega)}{(\omega-z)^{k+1}} d\omega, \quad |z| < \rho < r.$$

Let  $|z| = r - \delta$  and  $\omega = \rho e^{i\theta}$ . Then

$$|f^{(k)}(z)| \leq \frac{k! \rho}{2\pi} \int_{\theta=0}^{2\pi} \frac{|f(\rho e^{i\theta})|}{(\rho - r + \delta)^{k+1}} d\theta .$$

Integrating this inequality with respect to  $\rho$  from  $r - \delta\varphi$  to  $r$ , ( $0 < \varphi < 1$ ), we get

$$\begin{aligned}
|f^{(k)}(z)| \delta\varphi &\leq \frac{k!}{2\pi} \int_{\rho=r-\delta\varphi}^r \int_{\theta=0}^{2\pi} \frac{|f(\rho e^{i\theta})|}{(\varphi-r+\delta)^{k+1}} \rho d\rho d\theta \\
&\leq \frac{k!}{2\pi} \left\{ \int_{\rho=r-\delta\varphi}^r \int_{\theta=0}^{2\pi} \frac{\rho d\rho d\theta}{(\rho-r+\delta)^{2k+2}} \right\}^{1/2} \|f\|_{L^2(\hat{C}_r)}
\end{aligned}$$

Now let us evaluate the integral under the square root.

$$\begin{aligned}
&\int_{\rho=r-\delta\varphi}^r \int_{\theta=0}^{2\pi} \frac{\rho d\rho d\theta}{(\rho-r+\delta)^{2k+2}} \\
&= 2\pi \int_{\rho=r-\delta\varphi}^r \frac{\rho d\rho}{(\rho-r+\delta)^{2k+2}} \\
&= 2\pi \left[ \frac{1}{2k+1} \frac{r-\delta\varphi}{\{(1-\varphi)\delta\}^{2k+1}} - \frac{1}{2k+1} \frac{r}{\delta^{2k+1}} \right] \\
&\quad + 2\pi \left[ \frac{-1}{(2k+1)(2k)} \left\{ \frac{1}{(\rho-r+\delta)^{2k}} \right\} \right]_{\rho=r-\delta\varphi}^r \\
&= \frac{2\pi}{(2k+1)\delta^{2k+1}} \{ (r-\delta\varphi)(1-\varphi)^{-(2k+1)} - r \} \\
&\quad - \frac{2\pi}{(2k+1)(2k)\delta^{2k}} [ (1-\varphi)^{-2k} - 1 ] \\
&\leq \frac{2\pi r}{(2k+1)\delta^{2k+1}} \frac{1}{(1-\varphi)^{2k+1}}.
\end{aligned}$$

Choosing  $\varphi = \frac{1}{2}$ , we get

$$\begin{aligned}
|f^{(k)}(z)| \left(\frac{1}{2}\delta\right) &\leq \frac{k!}{2\pi} \sqrt{\frac{2\pi r}{(2k+1)} \left(\frac{2}{\delta}\right)^{2k+1}} \|f\|_{L^2(\hat{C}_r)} \\
&\leq k! \sqrt{\frac{r}{2\pi}} \left(\frac{2}{\delta}\right)^{k+1/2} \|f\|_{L^2(\hat{C}_r)}
\end{aligned}$$

Hence

$$||D_z^k|| \leq k! \left(\frac{r}{2\pi}\right)^{\frac{1}{2}} \left(\frac{2}{r-|z|}\right)^{k+3/2},$$

which proves the result.

#### 4.3 Quadrature Optimal Multistep Methods in $L^2(\hat{C}_r)$

The coefficients  $\tilde{b}_j$  in a quadrature optimal formula, in  $L^2(\hat{C}_r)$ ,

$$(4) \quad Y_{n+1} = Y_{n-s} + h \sum_{j=\delta_{to}}^m \tilde{b}_j f(x_{n+1-j}, Y_{n+1-j})$$

satisfy the normal equations

$$(5) \quad \tilde{C} \tilde{b} = \tilde{d}$$

with

$$\tilde{C}_{ij} = \frac{r^2}{\pi(r^2 - x_{n+1-j} \bar{x}_{n+1-i})^2},$$

and

$$\tilde{d}_i = \frac{r^2}{\pi h} \frac{x_{n+1} - x_{n-s}}{(r^2 - x_{n+1} \bar{x}_{n+1-i})(r^2 - x_{n-s} \bar{x}_{n+1-i})},$$

$$i, j = \delta_{to}(1)m.$$

The following theorem characterizes such a multistep formula.

Theorem 2. The quadrature optimal multistep formula (4) is characterized by that it is locally interpolatory for functions

$$y_i(x) = \begin{cases} (r^2 - \bar{x}_{n+1-i} x)^{-1} & , \text{ if } x_{n+1-i} \neq 0 \\ x & , \text{ if } x_{n+1-i} = 0 \end{cases}$$

$$i = \delta_{t_0}, 1, 2, \dots, m.$$

Proof. Proceeding as in the proof of Theorem 2.2 and making use of (2) we find that the formula (4) is interpolatory for the functions

$$y_i(x) = \begin{cases} -\frac{r^2}{\pi \bar{x}_{n+1-i}} \frac{1}{(r^2 - x \bar{x}_{n+1-i})} & , \text{ if } x_{n+1-i} \neq 0 \\ \frac{x}{\pi} & , \text{ if } x_{n+1-i} = 0, i = \delta_{t_0}(1)m, \end{cases}$$

from which the result follows.

It is worth noting that if  $r, h$  and  $x_{n+1-i}$  in the normal equations are respectively replaced by  $\alpha r, \alpha h$  and  $\alpha x_{n+1-i}$ , the normal equations do not change and hence the coefficients  $\tilde{b}_j$  remain the same. This implies that working with one value of  $r$  and calculating the coefficients  $\tilde{b}_j$  for different values of  $h$  is sufficient to give rise to the coefficients for different values of  $r$ . This observation is easily seen to be applicable to the methods of the previous chapters as well.

The  $L^2(\hat{C}_r)$ -norm of local truncation error functional  $T_n$  at point  $x_{n+1}$  for any multistep formula of quadrature type with coefficients  $b_j$  turns out to be given by



$$\begin{aligned}
(6) \quad ||\underline{T}_n||^2 &= \frac{r^2}{\pi} \left[ (r^2 - |x_{n+1}|^2)^{-2} + (r^2 - |x_{n-s}|^2)^{-2} \right. \\
&\quad - 2\operatorname{Re} \{ (r^2 - x_{n+1} \bar{x}_{n-s}) \}^{-1} - h \sum_{j=\delta_{to}}^m \underline{b}_j g(x_{n+1-j}) \\
&\quad - h \sum_{k=\delta_{to}}^m \bar{\underline{b}}_k \{ \overline{g(x_{n+1-k})} \} \\
&\quad \left. - 2h \sum_{j=\delta_{to}}^m \underline{b}_j \frac{r^2 + 2x_{n+1-j} \bar{x}_{n+1-i}}{(r^2 - x_{n+1-j} \bar{x}_{n+1-i})^4} \right] ,
\end{aligned}$$

where

$$g(x) = 2x \{ (r^2 - \bar{x}_{n+1}x)^{-3} - (r^2 - \bar{x}_{n-s}x)^{-3} \} .$$

In the numerical results to follow (5) and (6) have been implemented for  $L^2(\hat{c}_r)$  with  $r = 2.01$  and corresponding to the standard situation of  $h=.1$  with  $x_i = ih$ ,  $i=0, \pm 1, \dots$  of earlier chapters.

Table 4.1 displays the local truncation error norms and the coefficients of  $L^2(\hat{c}_r)$ -quadrature optimal  $(m=5)$  multistep formulae in the implicit and explicit cases. The general behaviour of coefficients has been the same as in the case of  $H^2(c_r)$  formulae. The range of variation of coefficients in the present case has however, slightly increased. At the point  $x = -1.5$  the error norm in the  $L^2(\hat{c}_r)$ -quadrature optimal case is about  $1/7500$  of the usual case. This indicates that the norm of local truncation error functional has reduced as compared to the  $H^2(c_r)$ -quadrature optimal case.

Table 4.1

SITUATION: Y' IN  $U^2(Cr)$ ; R = 2.01 H = .10  
MULTI STEP METHOD OF 5 STEPS

SITUATION: Y' IN L<sup>2</sup>(C<sup>2</sup>)

; R= 2.01 H= .10


$$L(C, r)$$

SITUATION: Y' IN

X	EUSUAL	EOPITAL	H X B(1)	H X B(2)	H X B(3)	H X B(4)	H X B(5)
0	0	0	0	0	0	0	0
1	0	0	0	0	0	0	0
2	0	0	0	0	0	0	0
3	0	0	0	0	0	0	0
4	0	0	0	0	0	0	0
5	0	0	0	0	0	0	0
6	0	0	0	0	0	0	0
7	0	0	0	0	0	0	0
8	0	0	0	0	0	0	0
9	0	0	0	0	0	0	0
10	0	0	0	0	0	0	0
11	0	0	0	0	0	0	0
12	0	0	0	0	0	0	0
13	0	0	0	0	0	0	0
14	0	0	0	0	0	0	0
15	0	0	0	0	0	0	0
16	0	0	0	0	0	0	0
17	0	0	0	0	0	0	0
18	0	0	0	0	0	0	0
19	0	0	0	0	0	0	0
20	0	0	0	0	0	0	0
21	0	0	0	0	0	0	0
22	0	0	0	0	0	0	0
23	0	0	0	0	0	0	0
24	0	0	0	0	0	0	0
25	0	0	0	0	0	0	0
26	0	0	0	0	0	0	0
27	0	0	0	0	0	0	0
28	0	0	0	0	0	0	0
29	0	0	0	0	0	0	0
30	0	0	0	0	0	0	0
31	0	0	0	0	0	0	0
32	0	0	0	0	0	0	0
33	0	0	0	0	0	0	0
34	0	0	0	0	0	0	0
35	0	0	0	0	0	0	0
36	0	0	0	0	0	0	0
37	0	0	0	0	0	0	0
38	0	0	0	0	0	0	0
39	0	0	0	0	0	0	0
40	0	0	0	0	0	0	0
41	0	0	0	0	0	0	0
42	0	0	0	0	0	0	0
43	0	0	0	0	0	0	0
44	0	0	0	0	0	0	0
45	0	0	0	0	0	0	0
46	0	0	0	0	0	0	0
47	0	0	0	0	0	0	0
48	0	0	0	0	0	0	0
49	0	0	0	0	0	0	0
50	0	0	0	0	0	0	0
51	0	0	0	0	0	0	0
52	0	0	0	0	0	0	0
53	0	0	0	0	0	0	0
54	0	0	0	0	0	0	0
55	0	0	0	0	0	0	0
56	0	0	0	0	0	0	0
57	0	0	0	0	0	0	0
58	0	0	0	0	0	0	0
59	0	0	0	0	0	0	0
60	0	0	0	0	0	0	0
61	0	0	0	0	0	0	0
62	0	0	0	0	0	0	0
63	0	0	0	0	0	0	0
64	0	0	0	0	0	0	0
65	0	0	0	0	0	0	0
66	0	0	0	0	0	0	0
67	0	0	0	0	0	0	0
68	0	0	0	0	0	0	0
69	0	0	0	0	0	0	0
70	0	0	0	0	0	0	0
71	0	0	0	0	0	0	0
72	0	0	0	0	0	0	0
73	0	0	0	0	0	0	0
74	0	0	0	0	0	0	0
75	0	0	0	0	0	0	0
76	0	0	0	0	0	0	0
77	0	0	0	0	0	0	0
78	0	0	0	0	0	0	0
79	0	0	0	0	0	0	0
80	0	0	0	0	0	0	0
81	0	0	0	0	0	0	0
82	0	0	0	0	0	0	0
83	0	0	0	0	0	0	0
84	0	0	0	0	0	0	0
85	0	0	0	0	0	0	0
86	0	0	0	0	0	0	0
87	0	0	0	0	0	0	0
88	0	0	0	0	0	0	0
89	0	0	0	0	0	0	0
90	0	0	0	0	0	0	0
91	0	0	0	0	0	0	0
92	0	0	0	0	0	0	0
93	0	0	0	0	0	0	0
94	0	0	0	0	0	0	0
95	0	0	0	0	0	0	0
96	0	0	0	0	0	0	0
97	0	0	0	0	0	0	0
98	0	0	0	0	0	0	0
99	0	0	0	0	0	0	0
100	0	0	0	0	0	0	0

X	EUSUAL	EOPITAL	H X B(1)	H X B(2)	H X B(3)	H X B(4)	H X B(5)
0	0	0	0	0	0	0	0
1	0	0	0	0	0	0	0
2	0	0	0	0	0	0	0
3	0	0	0	0	0	0	0
4	0	0	0	0	0	0	0
5	0	0	0	0	0	0	0
6	0	0	0	0	0	0	0
7	0	0	0	0	0	0	0
8	0	0	0	0	0	0	0
9	0	0	0	0	0	0	0
10	0	0	0	0	0	0	0
11	0	0	0	0	0	0	0
12	0	0	0	0	0	0	0
13	0	0	0	0	0	0	0
14	0	0	0	0	0	0	0
15	0	0	0	0	0	0	0
16	0	0	0	0	0	0	0
17	0	0	0	0	0	0	0
18	0	0	0	0	0	0	0
19	0	0	0	0	0	0	0
20	0	0	0	0	0	0	0
21	0	0	0	0	0	0	0
22	0	0	0	0	0	0	0
23	0	0	0	0	0	0	0
24	0	0	0	0	0	0	0
25	0	0	0	0	0	0	0
26	0	0	0	0	0	0	0
27	0	0	0	0	0	0	0
28	0	0	0	0	0	0	0
29	0	0	0	0	0	0	0
30	0	0	0	0	0	0	0
31	0	0	0	0	0	0	0
32	0	0	0	0	0	0	0
33	0	0	0	0	0	0	0
34	0	0	0	0	0	0	0
35	0	0	0	0	0	0	0
36	0	0	0	0	0	0	0
37	0	0	0	0	0	0	0
38	0	0	0	0	0	0	0
39	0	0	0	0	0	0	0
40	0	0	0	0	0	0	0
41	0	0	0	0	0	0	0
42	0	0	0	0	0	0	0
43	0	0	0	0	0	0	0
44	0	0	0	0	0	0	0
45	0	0	0	0	0	0	0
46	0	0	0	0	0	0	0
47	0	0	0	0	0	0	0
48	0	0	0	0	0	0	0
49	0	0	0	0	0	0	0
50	0	0	0	0	0	0	0
51	0	0	0	0	0	0	0
52	0	0	0	0	0	0	0
53	0	0	0	0	0	0	0
54	0	0	0	0	0	0	0
55	0	0	0	0	0	0	0
56	0	0	0	0	0	0	0
57	0	0	0	0	0	0	0
58	0	0	0	0	0	0	0
59	0	0	0	0	0	0	0
60	0	0	0	0	0	0	0
61	0	0	0	0	0	0	0
62	0	0	0	0	0	0	0
63	0	0	0	0	0	0	0
64	0	0	0	0	0	0	0
65	0	0	0	0	0	0	0
66	0	0	0	0	0	0	0
67	0	0	0	0	0	0	0
68	0	0	0	0	0	0	0
69	0	0	0	0	0	0	0
70	0	0	0	0	0	0	0
71	0	0	0	0	0	0	0
72	0	0	0	0	0	0	0
73	0	0	0	0	0	0	0
74	0	0	0	0	0	0	0
75	0	0	0	0	0	0	0
76	0	0	0	0	0	0	0
77	0	0	0	0	0	0	0
78	0	0	0	0	0	0	0
79	0	0	0	0	0	0	0
80	0	0	0	0	0	0	0
81	0	0	0	0	0	0	0
82	0	0	0	0	0	0	0
83	0	0	0	0	0	0	0
84	0	0	0	0	0	0	0
85	0	0	0	0	0	0	0
86	0	0	0	0	0	0	0
87	0	0	0	0	0	0	0
88	0	0	0	0	0	0	0
89	0	0	0	0	0	0	0
90	0	0	0	0	0	0	0
91	0	0	0	0	0	0	0
92	0	0	0	0	0	0	0
93	0	0	0	0	0	0	0
94	0	0	0	0	0	0	0
95	0	0	0	0	0	0	0
96	0	0	0	0	0	0	0
97	0	0	0	0	0	0	0
98	0	0	0	0	0	0	0
99	0	0	0	0	0	0	0
100	0	0	0	0	0	0	0

X	EUSUAL	EOPITAL	H X B(1)	H X B(2)	H X B(3)	H X B(4)	H X B(5)
0	0	0	0	0	0	0	0
1	0	0	0	0	0	0	0
2	0	0	0	0	0	0	0
3	0	0	0	0	0	0	0
4	0	0	0	0	0	0	0
5	0	0	0	0	0	0	0
6	0	0	0	0	0	0	0
7	0	0	0	0	0	0	0
8	0	0	0	0	0	0	0
9	0	0	0	0	0	0	0
10	0	0	0	0	0	0	0
11	0	0	0	0	0	0	0
12	0	0	0	0	0	0	0
13	0	0	0	0	0	0	0
14	0	0	0	0	0	0	0
15	0	0	0	0	0	0	0
16	0	0	0	0	0	0	0
17	0	0	0	0	0	0	0
18	0	0	0	0	0	0	0
19	0	0	0	0	0	0	0
20	0	0	0	0	0	0	0
21	0	0	0	0	0	0	0
22	0	0	0	0	0	0	0
23	0	0	0	0	0	0	0
24	0	0	0	0	0	0	0
25	0	0	0	0	0	0	0
26	0	0	0	0	0	0	0
27	0	0	0	0	0	0	0
28							

Table 4.1(a)

[illegible]

Table 4.1(b)

[illegible]

Table 4.1(c)

DIFFERENTIAL EQUATION NO. 13										DIFFERENTIAL EQUATION NO. 14										DIFFERENTIAL EQUATION NO. 15										DIFFERENTIAL EQUATION NO. 16									
X	Y(X)	EIO	FEU	ITU	X	Y(X)	EIO	FEU	ITU	X	Y(X)	EIO	FEU	ITU	X	Y(X)	EIO	FEU	ITU																				
1	0.000																																						

Table 4.1(d)

[illegible]



Tables 4.1(a)-4.1(d) are applications of Table 4.1 on the set of twenty four differential equations. The  $L^2(c_r)$ -explicit quadrature optimal 5-step method has performed just better on equations 14, 16 and 24; one decimal place better on equations 2, 4, 6, 8, 11, 12, 13, 15, 17, 18, 19, 20, and 23 and two decimal places better on equations 1, 3, 5, 7, 9, 10, 21 and 22 as compared to the usual method. The implicit quadrature optimal method has been one decimal place better on equations 3, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23 and 24; two decimal places better on equations 1, 4, 5, 6, 7, 8, 9 and 10; and three decimal places better on equation 2, as compared with the corresponding usual implicit method.

#### 4.4 Quadrature Optimal Multistep Methods in $L^2(\hat{c}_r)$ Interpolatory for Polynomials

As in Section 2.4, for equidistant points  $x_{n+1-i}$ , the coefficients  $\tilde{\gamma}_j^p$  of a  $L^2(\hat{c}_r)$ -quadrature optimal multistep formula

$$\begin{aligned}
 (7) \quad y_{n+1} - y_{n-s} - h \sum_{j=0}^{p-1} \gamma_j^u \nabla^j f(x_{n+\delta_{t1}}, y_{n+\delta_{t1}}) \\
 = h \sum_{j=p}^{m-\delta_{t0}} \tilde{\gamma}_j^p \nabla^j f(x_{n+\delta_{t1}}, y_{n+\delta_{t1}}),
 \end{aligned}$$

interpolatory for polynomials of degree  $p < m + \delta_{t1}$ , are similarly to satisfy the normal equations

$$(8) \quad \tilde{C} \tilde{\gamma}^P = \tilde{d}^P,$$

where, for  $i, j = p(1)m - \delta_{t_0}$ ,

$$\tilde{\gamma}^P = (\tilde{\gamma}_p^P, \dots, \tilde{\gamma}_{m-\delta_{t_0}}^P)^T,$$

$$l_{ij}^P = \frac{r^2}{\pi} \sum_{k=0}^j \sum_{l=0}^i (-1)^{l+k} \binom{i}{l} \binom{j}{k} \frac{1}{(r^2 - x_{n+\delta_{t_1}} - k \bar{x}_{n+\delta_{t_1}} - l)^2}$$

and

$$\begin{aligned} l_i^P &= \frac{r^2}{\pi h} \left[ \sum_{l=0}^i (-1)^l \binom{i}{l} \frac{x_{n+1} - x_{n-s}}{(r^2 - x_{n+1} \bar{x}_{n+\delta_{t_1}} - l)(r^2 - x_{n-s} \bar{x}_{n+\delta_{t_1}} - l)} \right] \\ &\quad - \frac{r^2}{\pi} \sum_{q=0}^{p-1} \gamma_q^u \left\{ \sum_{k=0}^q \sum_{l=0}^i (-1)^{l+k} \binom{i}{l} \binom{q}{k} \right. \\ &\quad \left. \frac{1}{(r^2 - x_{n+\delta_{t_1}} - k \bar{x}_{n+\delta_{t_1}} - l)^2} \right\} \end{aligned}$$

The following theorem characterizes formula (7).

Theorem 3: The multistep formula (7) is a quadrature optimal formula if, and only if, it is locally interpolatory for the  $m - p + \delta_{t_1}$  functions

$$h_j(x) = \sum_{k=0}^j (-1)^k \binom{j}{k} \left\{ \frac{1}{\bar{x}_{n+\delta_{t_1}} - k} \frac{1}{(r^2 - \bar{x}_{n+\delta_{t_1}} - kx)} \right\}^*,$$

$$j = p(1)m - \delta_{t_0},$$

where  $\{ \cdot \}^*$  is to be replaced by  $x/r^2$  if  $x_{n+\delta_{t_1}} - k = 0$ .

The proof which uses (2) and is similar to that of Theorem 2.3 is omitted.



The multistep coefficients  $\tilde{b}_j^p$  in the following numerical results are obtained from the coefficients  $\gamma_j^u$  and  $\tilde{\gamma}_j^p$  as determined through (8).

In Tables 4.2 to 4.6 the coefficients and error norms of  $L^2(\hat{C}_r)$ -quadrature optimal 5-step methods interpolatory for polynomials of degree  $1 \leq p \leq 5$  are displayed. A summary of numerical results obtained by applying these methods on the set of twenty four differential equations is as follows:

As compared with the usual explicit cases the  $L^2(\hat{C}_r)$ -quadrature optimal 5-step method with  $p=1$  has worked just better on equations 13, 14 and 24; one decimal place better on equations 2, 6, 8, 10, 11, 12, 15, 16, 17, 18, 19 and 23; and two decimal places better on equations 1, 3, 4, 5, 7, 9, 20, 21 and 22. In the implicit case the method has worked just better on equations 14 and 24; one decimal place better on equations 3, 11, 12, 13, 15, 16, 17, 18, 19, 20, 21, 22 and 23; and two decimal places better on equation 2.

The explicit method with  $p=2$  performed just better on equations 13, 14, 16 and 24; one decimal place better on equations 2, 6, 8, 10, 11, 12, 15, 17, 18, 19 and 23; and two decimal places better on equations 1, 3, 4, 5, 7, 9, 20, 21 and 22. The implicit method has been just better on equations 12, 18 and 24; one decimal place better on equations

[illegible]

SITUATION: Y' IN  $\bar{L}(C, r)$ ; R = 2.01 H = .10  
MULTI STEP METHOD OF 5 STEPS INTERPOLATRY UPTO 2 DEGREE POLYNOMIALS

[illegible]

## Table 4.4

[illegible]

Table 4.5

SITUATION:  $y'$  IN  $L(C, r)$ !  $R = 2.01$  H = 10  
MULTI STEP METHOD OF 5 STEPS INTERPOLATION UP

X	EUSUAL	EOPTIMAL	H X B(1)	H X B(2)	H X B(3)	H X B(4)	H X B(5)
1	3	1	0	0	0	0	0
2	1	1	0	0	0	0	0
3	1	1	0	0	0	0	0
4	1	1	0	0	0	0	0
5	1	1	0	0	0	0	0
6	1	1	0	0	0	0	0
7	1	1	0	0	0	0	0
8	1	1	0	0	0	0	0
9	1	1	0	0	0	0	0
10	1	1	0	0	0	0	0
11	1	1	0	0	0	0	0
12	1	1	0	0	0	0	0
13	1	1	0	0	0	0	0
14	1	1	0	0	0	0	0
15	1	1	0	0	0	0	0
16	1	1	0	0	0	0	0
17	1	1	0	0	0	0	0
18	1	1	0	0	0	0	0
19	1	1	0	0	0	0	0
20	1	1	0	0	0	0	0
21	1	1	0	0	0	0	0
22	1	1	0	0	0	0	0
23	1	1	0	0	0	0	0
24	1	1	0	0	0	0	0
25	1	1	0	0	0	0	0
26	1	1	0	0	0	0	0
27	1	1	0	0	0	0	0
28	1	1	0	0	0	0	0
29	1	1	0	0	0	0	0
30	1	1	0	0	0	0	0
31	1	1	0	0	0	0	0
32	1	1	0	0	0	0	0
33	1	1	0	0	0	0	0
34	1	1	0	0	0	0	0
35	1	1	0	0	0	0	0
36	1	1	0	0	0	0	0
37	1	1	0	0	0	0	0
38	1	1	0	0	0	0	0
39	1	1	0	0	0	0	0
40	1	1	0	0	0	0	0
41	1	1	0	0	0	0	0
42	1	1	0	0	0	0	0
43	1	1	0	0	0	0	0
44	1	1	0	0	0	0	0
45	1	1	0	0	0	0	0
46	1	1	0	0	0	0	0
47	1	1	0	0	0	0	0
48	1	1	0	0	0	0	0
49	1	1	0	0	0	0	0
50	1	1	0	0	0	0	0
51	1	1	0	0	0	0	0
52	1	1	0	0	0	0	0
53	1	1	0	0	0	0	0
54	1	1	0	0	0	0	0
55	1	1	0	0	0	0	0
56	1	1	0	0	0	0	0
57	1	1	0	0	0	0	0
58	1	1	0	0	0	0	0
59	1	1	0	0	0	0	0
60	1	1	0	0	0	0	0
61	1	1	0	0	0	0	0
62	1	1	0	0	0	0	0
63	1	1	0	0	0	0	0
64	1	1	0	0	0	0	0
65	1	1	0	0	0	0	0
66	1	1	0	0	0	0	0
67	1	1	0	0	0	0	0
68	1	1	0	0	0	0	0
69	1	1	0	0	0	0	0
70	1	1	0	0	0	0	0
71	1	1	0	0	0	0	0
72	1	1	0	0	0	0	0
73	1	1	0	0	0	0	0
74	1	1	0	0	0	0	0
75	1	1	0	0	0	0	0

X	EUSUAL	EOPTIMAL	H X B(0)	H X B(1)	H X B(2)	H X B(3)	H X B(4)	H X B(5)
1	3	1	0	0	0	0	0	0
2	1	1	0	0	0	0	0	0
3	1	1	0	0	0	0	0	0
4	1	1	0	0	0	0	0	0
5	1	1	0	0	0	0	0	0
6	1	1	0	0	0	0	0	0
7	1	1	0	0	0	0	0	0
8	1	1	0	0	0	0	0	0
9	1	1	0	0	0	0	0	0
10	1	1	0	0	0	0	0	0
11	1	1	0	0	0	0	0	0
12	1	1	0	0	0	0	0	0
13	1	1	0	0	0	0	0	0
14	1	1	0	0	0	0	0	0
15	1	1	0	0	0	0	0	0
16	1	1	0	0	0	0	0	0
17	1	1	0	0	0	0	0	0
18	1	1	0	0	0	0	0	0
19	1	1	0	0	0	0	0	0
20	1	1	0	0	0	0	0	0
21	1	1	0	0	0	0	0	0
22	1	1	0	0	0	0	0	0
23	1	1	0	0	0	0	0	0
24	1	1	0	0	0	0	0	0
25	1	1	0	0	0	0	0	0
26	1	1	0	0	0	0	0	0
27	1	1	0	0	0	0	0	0
28	1	1	0	0	0	0	0	0
29	1	1	0	0	0	0	0	0
30	1	1	0	0	0	0	0	0
31	1	1	0	0	0	0	0	0
32	1	1	0	0	0	0	0	0
33	1	1	0	0	0	0	0	0
34	1	1	0	0	0	0	0	0
35	1	1	0	0	0	0	0	0
36	1	1	0	0	0	0	0	0
37	1	1	0	0	0	0	0	0
38	1	1	0	0	0	0	0	0
39	1	1	0	0	0	0	0	0
40	1	1	0	0	0	0	0	0
41	1	1	0	0	0	0	0	0
42	1	1	0	0	0	0	0	0
43	1	1	0	0	0	0	0	0
44	1	1	0	0	0	0	0	0
45	1	1	0	0	0	0	0	0
46	1	1	0	0	0	0	0	0
47	1	1	0	0	0	0	0	0
48	1	1	0	0	0	0	0	0
49	1	1	0	0	0	0	0	0
50	1	1	0	0	0	0	0	0
51	1	1	0	0	0	0	0	0
52	1	1	0	0	0	0	0	0
53	1	1	0	0	0	0	0	0
54	1	1	0	0	0	0	0	0
55	1	1	0	0	0	0	0	0
56	1	1	0	0	0	0	0	0
57	1	1	0	0	0	0	0	0
58	1	1	0	0	0	0	0	0
59	1	1	0	0	0	0	0	0
60	1	1	0	0	0	0	0	0
61	1	1	0	0	0	0	0	0
62	1	1	0	0	0	0	0	0
63	1	1	0	0	0	0	0	0
64	1	1	0	0	0	0	0	0
65	1	1	0	0	0	0	0	0
66	1	1	0	0	0	0	0	0
67	1	1	0	0	0	0	0	0
68	1	1	0	0	0	0	0	0
69	1	1	0	0	0	0	0	0
70	1	1	0	0	0	0	0	0
71	1	1	0	0	0	0	0	0
72	1	1	0	0	0	0	0	0
73	1	1	0	0	0	0	0	0
74	1	1	0	0	0	0	0	0
75	1	1	0	0	0	0	0	0



11,12,13,14,15,16,19,20,21, 22 and 23, and two decimal places better on equations 1,2,3,4,5,6,7,8,9 and 10.

The explicit method with  $p=3$  has been just better on equations 11,12,13,14,16 and 24; one decimal place better on equations 1,2,3,5,6,8,9,10,15,19,20,22 and 23; and two decimal places better on equations 4,7, and 21. The implicit method with  $p=3$  has been just better on equations 11,12 and 24; one decimal place better on equations 3,10,13,14,15,16,19,20,21,22 and 23 and two decimal places better on equations 1,2,4,5,6,7,8 and 9. The two methods have been comparable on equations 17 and 18.

The explicit method with  $p=4$  has been just better on equations 14,17,18 and 24; one decimal place better on equations 1, 2,3,6,7,8,9,10,13,15,16,19,20,22 and 23 and 2 decimal places better on equation 9. The implicit method with  $p=4$  has been just better on equations 15,17, 18 and 24; one decimal place better on equations 1,2,3,4, 5,6,7,8,10,13,14,16,19,20,21,22 and 23; and two decimal places better on equation 9. The methods have been just worse on equations 11 and 12.

The implicit method with  $p=5$  has been just better on equations 10,13,15,16,17 and 18; one decimal place better on equations 1,2,3,5,6,7,8,14,19,20,21,22,23 and 24 and two decimal places better on equations 4 and 9.

#### 4.5 Quadrature Optimal Multistep Methods in $L^2(\hat{C}_r)$ Interpolatory for a Set of Preassigned Functions

The coefficients  $\tilde{b}_j^F$  of a quadrature optimal multistep formula in  $L^2(\hat{C}_r)$

$$(9) \quad Y_{n+1} - Y_{n-s} = h \sum_{j=\delta_{to}}^m \tilde{b}_j^F f(x_{n+1-j}, Y_{n+1-j}),$$

interpolatory for linearly independent functions

$\{\varphi_1, \dots, \varphi_p\}$ , are to satisfy normal equations

$$\begin{bmatrix} \tilde{C} & F^* \\ F & 0 \end{bmatrix} \begin{bmatrix} \tilde{b}^F \\ \lambda \end{bmatrix} = \begin{bmatrix} \tilde{d} \\ e \end{bmatrix},$$

where  $\tilde{C}$ ,  $\tilde{d}$  are as in equations (5),  $\tilde{b}^F = [\tilde{b}_{to}^F, \dots, \tilde{b}_m^F]$ ,  $\lambda = [\lambda_1, \dots, \lambda_p]^T$ ,

$$F = [\varphi_i^1(x_{n+1-j})]_{i=1, j=\delta_{to}}^{p, m},$$

$$e_i = \varphi_i(x_{n+1}) - \varphi_i(x_{n-s}), \quad i=1(1)p,$$

and 0 is  $p \times p$  null matrix. Here we have:

**Theorem 4:** A quadrature optimal multistep method in  $L^2(\hat{C}_r)$  interpolatory for functions  $\{\varphi_1, \dots, \varphi_p\}$  is characterized by that it is locally interpolatory for constants and functions

$$\{\varphi_1, \dots, \varphi_p\} \cup \{h_k(x), k = p + \delta_{to}(1)m\},$$

where



$$\begin{aligned}
 \underline{h}_k(x) = & \left[ \{ \bar{x}_{n+1-k} (r^2 - \bar{x}_{n+1-k} x) \}^{-1} \right]_* \\
 & + \sum_{j=\delta_{to}}^{p-1+\delta_{to}} \left\{ \sum_{q=\delta_{to}}^{p-1+\delta_{to}} \bar{\omega}_{j+1-\delta_{to}, q} \bar{\varphi}'_{q+1-\delta_{to}}(x_{n+1-k}) \right\} \cdot \\
 & \cdot \left[ \{ \bar{x}_{n+1-j} (r^2 - \bar{x}_{n+1-j} x) \}^{-1} \right]_* ,
 \end{aligned}$$

where

$$W = [\omega_{ij}]_{\substack{i=1(1)p \\ j=\delta_{to}(1)p-1+\delta_{to}}}$$

with

$$W^{-1} = [\varphi'_i(x_{n+1-j})]_{\substack{j=1(1)p \\ j=\delta_{to}(1)p-1+\delta_{to}}}$$

and \* under the bracket means that the expression within is to be replaced by  $\frac{x}{r^2}$  if  $x_{n+1-l}=0$  for  $l=k$  or  $l=j$ .

Proof. The proof is immediate from Theorem 1.3 using (2) after simplifications.

In Table 4.7 we display the local truncation error norms for  $L_2(\hat{C}_r)$ -quadrature optimal multistep explicit and implicit methods interpolatory for functions  $\varphi_1(x) = \exp(1.6x)$  and  $\varphi_2(x) = \exp(-1.6x)$  and the coefficients of the methods. The general behaviour of the coefficients has been as earlier. The numerical results obtained by applying the coefficients of Table 2.7 on the set of twenty four differential equations are summarized as follows:

SITUATION:  $Y'$  IN  $L(Cr)$ ;  $R = 2.01$   $H = .10$ .

SITUATION: Y' IN L(C,r); R=2.01 H=.10  
FOR FYP( ALPHA\*X). ALPHA = 1.6 ALPHA = -1.6

[illegible]

As compared to explicit usual method the explicit quadrature optimal method has performed just better on equations 13,14,15 and 24; one decimal place better on equations 2,3,6,8,9,10,11,12,16,17,18,19 and 23; and two decimal places better on equations 1,4,5,7,20,21 and 22. The implicit quadrature optimal method has performed just better on equations 11,12,17,18 and 24; one decimal place better on equations 3,19,20,21,22 and 23; and two decimal places better on equations 1,2,4,5,6,7,8,9,10,13,14,15 and 16, in comparison with the corresponding usual implicit method.

#### 4.6 Limiting Behaviour of the Coefficients as $r \rightarrow \infty$

In Section 2.6 we studied a limiting behaviour, as  $r \rightarrow \infty$ , of the coefficients in quadrature optimal multistep formula for the space  $H^2(c_r)$ . Analogues of the results obtained therein also remain true for the space  $L^2(\hat{c}_r)$  with little change in the proofs. Accordingly, in this section we merely include the statements of the  $L^2(\hat{c}_r)$  results and omit their proofs, the only essential difference being that instead of the orthonormal basis  $\{\Psi_k\}$  as defined in (2.3) for  $H^2(c_r)$ , one is now to use the basis  $\{\underline{\Psi}_k\}$  of  $L^2(\hat{c}_r)$  as defined in (3) of this chapter.

Theorem 5: Let

$$Y_{n+1} = Y_{n-s} + h \sum_{j=\delta_{t0}}^m b_j^F f(x_{n+1-j}, Y_{n+1-j})$$

be a quadrature type usual multistep formula interpolatory for functions  $\{\varphi_{\delta_{t0}}, \dots, \varphi_m\}$  and let the matrix  $[\varphi'_i(x_{n+1-j})]_{i,j=\delta_{t0}}^m$  be non-singular. Let

$$(10) \quad Y_{n+1} = Y_{n-s} + h \sum_{j=\delta_{t0}}^m \tilde{b}_{jr}^F f(x_{n+1-j}, Y_{n+1-j})$$

be the quadrature optimal multistep formula in  $L^2(\hat{C}_r)$  interpolatory for functions  $\{\varphi_{\delta_{t0}}, \dots, \varphi_{p-1+\delta_{t0}}\}$ ,  $0 \leq p \leq m - \delta_{t0}$  ( $p=0$  meaning a non-interpolatory case). If the quadrature error  $\tilde{Q}_{nr}^F$  for (10) satisfies

$$\lim_{r \rightarrow \infty} \tilde{Q}_{nr}^F(\varphi_i) = 0, \quad i = p + \delta_{t0}(1)m,$$

then

$$\lim_{r \rightarrow \infty} \tilde{b}_{jr}^F = b_j^F, \quad j = \delta_{t0}(1)m.$$

Theorem 6: In  $L^2(\hat{C}_r)$ , the coefficients  $\tilde{b}_j$  of a quadrature optimal multistep formula (4) approach the coefficients of the corresponding usual formula as  $r \rightarrow \infty$ .

Theorem 7: In  $L^2(\hat{C}_r)$ , the coefficients  $\tilde{b}_{jr}^P$  of a quadrature optimal multistep formula

$$Y_{n+1} = Y_{n-s} + h \sum_{j=\delta_{t_0}}^m \tilde{b}_{jr}^P f(x_{n+1-j}, Y_{n+1-j}),$$

interpolatory for polynomials of degree  $p < m+1-\delta_{t_0}$ , approach the coefficients of the corresponding usual formula as  $r \rightarrow \infty$ .

Theorem 8: If the  $(m+\delta_{t_1}) \times (m+\delta_{t_1})$  matrix

$$M = \begin{bmatrix} \varphi_1'(x_{n+\delta_{t_1}}) & \dots & \varphi_1'(x_{n+1-m}) \\ \vdots & & \\ \varphi_p'(x_{n+\delta_{t_1}}) & \dots & \varphi_p'(x_{n+1-m}) \\ 1, & \dots & 1 \\ x_{n+\delta_{t_1}} & \dots & x_{n+1-m} \\ \vdots & & \\ x_{n+\delta_{t_1}}^{m-p-\delta_{t_0}} & \dots & x_{n+1-m}^{m-p-\delta_{t_0}} \end{bmatrix}$$

is non-singular, then, as  $r \rightarrow \infty$ , the coefficients  $\tilde{b}_{jr}^F$  of the quadrature optimal multistep formula

$$Y_{n+1} = Y_{n-s} + h \sum_{j=\delta_{t_0}}^m \tilde{b}_{jr}^F f(x_{n+1-j}, Y_{n+1-j}),$$

in  $L^2(\hat{C}_r)$ , interpolatory for functions  $\{\varphi_1(x) \dots \varphi_p(x)\}$ , approach the coefficients of the corresponding unique multistep formula

$$Y_{n+1} = Y_{n-s} + h \sum_{j=\delta_{t_0}}^m b_j^F f(x_{n+1-j}, Y_{n+1-j}),$$

interpolatory for  $\{\varphi_1(x), \dots, \varphi_p(x), x, x^2, \dots, x^{m-p+\delta_{t_1}}\}$ .

#### 4.7 Comparison of Different Methods

In Table 4.8 we present end point ( $x_N=1.2$ ) results obtained for quadrature optimal methods in  $L^2(\dot{C}_r)$  of one to four steps and compare these with the corresponding usual methods. We observe that the quadrature optimal methods have invariably remained better than the usual methods except in the case of equation 24.

In Figure 4.1 we have plotted  $\log_{10}(\|\tilde{T}_n(x)\|)$  and  $\log_{10}(\|T_n(x)\|)$  for the explicit methods. In Figure 4.2 the same is done for the implicit situation. We observe that the general behaviour of the errors is same as in the case of  $H^2(C_r)$  situation of Chapter 2.

In Table 4.9 we display end point ( $x_N=1.2$ ) errors for the set of twenty four differential equations corresponding to usual, quadrature optimal  $\tilde{M}$ , quadrature optimal methods interpolatory for polynomials of degrees 1 to 4 (denoted as  $\tilde{M}^1 \dots \tilde{M}^4$ ) and quadrature optimal method interpolatory for  $\exp(\pm 1.6x)$  (denoted as  $\tilde{M}^F$ ) for the explicit case. We observe that the errors are least for  $\tilde{M}$  on equations 3,4,6,8,19 and 22; for  $\tilde{M}^1$  on equations 6,11 and 12; for  $\tilde{M}^2$  on 1,2,3,4,6,10,15,16,17 and 18; for  $\tilde{M}^3$  on equation 23; for  $\tilde{M}^4$  on equations 5 and 24; and for  $\tilde{M}^F$  on equations 13,14,20 and 21. From Table 4.10, where we present the corresponding implicit situation, we observe that the

Table 4.8

SITUATION:  $Y'$  IN  $L^2(C, r)$ ;  $R = 2.01$   $H = .10$   
 ERRORS AT END POINT FOR EXPLICIT METHODS

Eq. No.	M	1		2		3		4	
		USUAL	OPTIMAL	USUAL	OPTIMAL	USUAL	OPTIMAL	USUAL	OPTIMAL
1.		-0.41E-01	-0.32E-01	0.25E-02	0.26E-03	-0.30E-02	-0.87E-03	0.17E-02	-0.42E-04
2.		-0.32E-01	-0.25E-01	0.16E-02	0.29E-04	-0.17E-02	-0.53E-03	0.75E-03	-0.63E-05
3.		-0.50E-01	-0.41E-01	0.43E-02	0.82E-03	-0.64E-02	-0.92E-03	0.30E-02	-0.19E-04
4.		-0.19E-01	-0.31E-01	0.28E-02	0.36E-03	-0.33E-02	-0.17E-03	0.17E-02	-0.32E-04
5.		-0.12E+00	-0.91E-01	-0.46E-02	0.25E-03	-0.50E-02	-0.17E-02	-0.22E-02	0.40E-04
6.		-0.44E-02	-0.36E-02	0.57E-03	0.11E-03	-0.69E-03	-0.15E-03	0.54E-03	-0.28E-04
7.		-0.56E-03	-0.42E-03	0.96E-04	0.23E-04	-0.11E-03	-0.11E-04	0.85E-04	-0.53E-05
8.		-0.67E-02	-0.65E-02	0.84E-03	0.64E-04	-0.94E-03	-0.68E-04	0.51E-03	-0.25E-04
9.		-0.20E-02	-0.16E-02	0.34E-03	0.66E-04	-0.37E-03	-0.11E-04	0.22E-03	-0.13E-04
10.		-0.17E+01	-0.15E+01	0.17E+00	0.17E+01	-0.21E+00	-0.51E+01	0.61E-01	-0.17E-02
11.		-0.13E+04	-0.88E+03	0.17E+03	0.12E+03	-0.39E+03	-0.13E+02	0.99E+02	-0.48E+01
12.		-0.13E+04	-0.76E+03	0.18E+03	0.81E+03	-0.17E+03	-0.96E+03	0.23E+04	-0.92E+05
13.		-0.99E-02	-0.71E-02	0.14E-03	0.14E-04	-0.13E-03	-0.88E-04	0.18E-04	-0.64E-05
14.		-0.85E-02	-0.60E-02	0.20E-03	0.20E-04	-0.13E-03	-0.88E-04	0.18E-04	-0.64E-05
15.		-0.80E-02	-0.59E-02	0.16E-03	0.16E-04	-0.11E-03	-0.88E-04	0.18E-04	-0.64E-05
16.		-0.67E-05	-0.55E-05	0.82E-06	0.71E-07	-0.73E-06	-0.66E-07	0.12E-06	-0.17E-07
17.		-0.66E-04	-0.54E-04	0.79E-05	0.92E-06	-0.69E-05	-0.59E-06	0.85E-06	-0.17E-07
18.		-0.63E-01	-0.53E-01	0.53E-02	0.42E-02	-0.63E-02	-0.55E-03	0.77E-03	-0.90E-04
19.		-0.60E-02	-0.53E-02	0.54E-03	0.44E-03	-0.63E-03	-0.55E-04	0.77E-04	-0.92E-05
20.		-0.57E-02	-0.53E-02	0.72E-03	0.53E-03	-0.72E-03	-0.63E-04	0.93E-04	-0.16E-05
21.		-0.22E+01	-0.18E+01	0.28E-02	0.28E-03	-0.33E-02	-0.46E-03	0.18E-02	-0.17E-03
22.		-0.26E+00	-0.18E+00	0.36E-02	0.36E-03	-0.44E-02	-0.63E-03	0.18E-02	-0.17E-03
23.		-0.22E-04	-0.23E-04	0.65E-04	0.32E-03	-0.77E-04	-0.13E-03	0.53E-04	-0.17E-04
24.		0.97E-04	0.23E-02	0.65E-04	0.32E-03	0.77E-04	0.13E-03	0.53E-04	-0.17E-04

ERRORS AT END POINT FOR IMPLICIT METHODS

Eq. No.	M	1		2		3		4	
		USUAL	OPTIMAL	USUAL	OPTIMAL	USUAL	OPTIMAL	USUAL	OPTIMAL
1.		-0.19E-03	-0.49E-04	0.27E-03	0.96E-04	-0.58E-04	-0.23E-05	0.69E-04	0.47E-05
2.		-0.12E-03	-0.22E-04	0.16E-03	0.60E-04	-0.28E-04	-0.15E-07	0.27E-04	0.22E-05
3.		-0.33E-03	-0.11E-03	0.43E-03	0.17E-03	-0.11E-03	-0.80E-05	0.14E-03	0.98E-05
4.		-0.09E-03	-0.58E-04	0.30E-03	0.10E-03	-0.62E-04	-0.23E-05	0.60E-04	0.44E-05
5.		-0.43E-04	-0.41E-04	0.58E-04	0.16E-03	-0.17E-04	-0.15E-05	0.21E-04	0.12E-05
6.		-0.79E-05	-0.15E-04	0.94E-05	0.24E-03	-0.28E-05	-0.29E-06	0.34E-05	0.19E-06
7.		-0.17E-04	-0.31E-05	0.09E-04	0.49E-05	-0.19E-04	-0.33E-05	0.22E-05	0.15E-06
8.		-0.28E-04	-0.17E-04	0.33E-04	0.11E-04	-0.25E-04	-0.83E-05	0.20E-04	0.17E-05
9.		-0.11E-01	-0.33E-02	0.22E-01	0.61E-02	-0.25E-02	-0.83E-04	0.13E+01	0.45E-01
10.		-0.11E+03	-0.48E+02	0.22E+02	0.13E+01	-0.60E+01	-0.55E+01	0.69E+06	0.37E+02
11.		-0.11E+03	-0.50E+02	0.22E+02	0.13E+01	-0.60E+01	-0.55E+01	0.69E+06	0.37E+02
12.		-0.11E+03	-0.44E-05	0.18E-04	0.09E-04	-0.11E-04	-0.68E-06	0.45E-06	0.33E-06
13.		-0.11E+03	-0.43E-05	0.14E-04	0.09E-04	-0.11E-04	-0.68E-06	0.45E-06	0.33E-06
14.		-0.11E+03	-0.22E-05	0.20E-04	0.09E-04	-0.11E-04	-0.68E-06	0.45E-06	0.33E-06
15.		-0.11E+03	-0.14E-05	0.16E-04	0.09E-04	-0.11E-04	-0.68E-06	0.45E-06	0.33E-06
16.		-0.77E-07	-0.14E-06	0.76E-07	0.74E-07	-0.46E-07	-0.88E-08	0.82E-07	0.23E-08
17.		-0.77E-06	-0.14E-06	0.76E-06	0.74E-06	-0.46E-06	-0.88E-07	0.82E-06	0.23E-07
18.		-0.28E-03	-0.32E-04	0.66E-03	0.19E-03	-0.13E-03	-0.62E-04	0.62E-04	0.14E-05
19.		-0.28E-03	-0.32E-04	0.66E-03	0.19E-03	-0.13E-03	-0.62E-04	0.62E-04	0.14E-05
20.		-0.63E-04	-0.57E-04	0.57E-04	0.24E-04	-0.63E-04	-0.55E-04	0.77E-04	-0.90E-05
21.		-0.63E-04	-0.57E-04	0.57E-04	0.24E-04	-0.63E-04	-0.55E-04	0.77E-04	-0.90E-05
22.		-0.32E-03	-0.18E-03	0.34E-03	0.52E-03	-0.33E-03	-0.93E-04	0.18E-03	-0.28E-04
23.		-0.32E-03	-0.18E-03	0.34E-03	0.52E-03	-0.33E-03	-0.93E-04	0.18E-03	-0.28E-04
24.		0.46E-06	0.27E-04	0.11E-04	0.13E-04	0.19E-05	0.34E-05	0.17E-05	0.28E-05

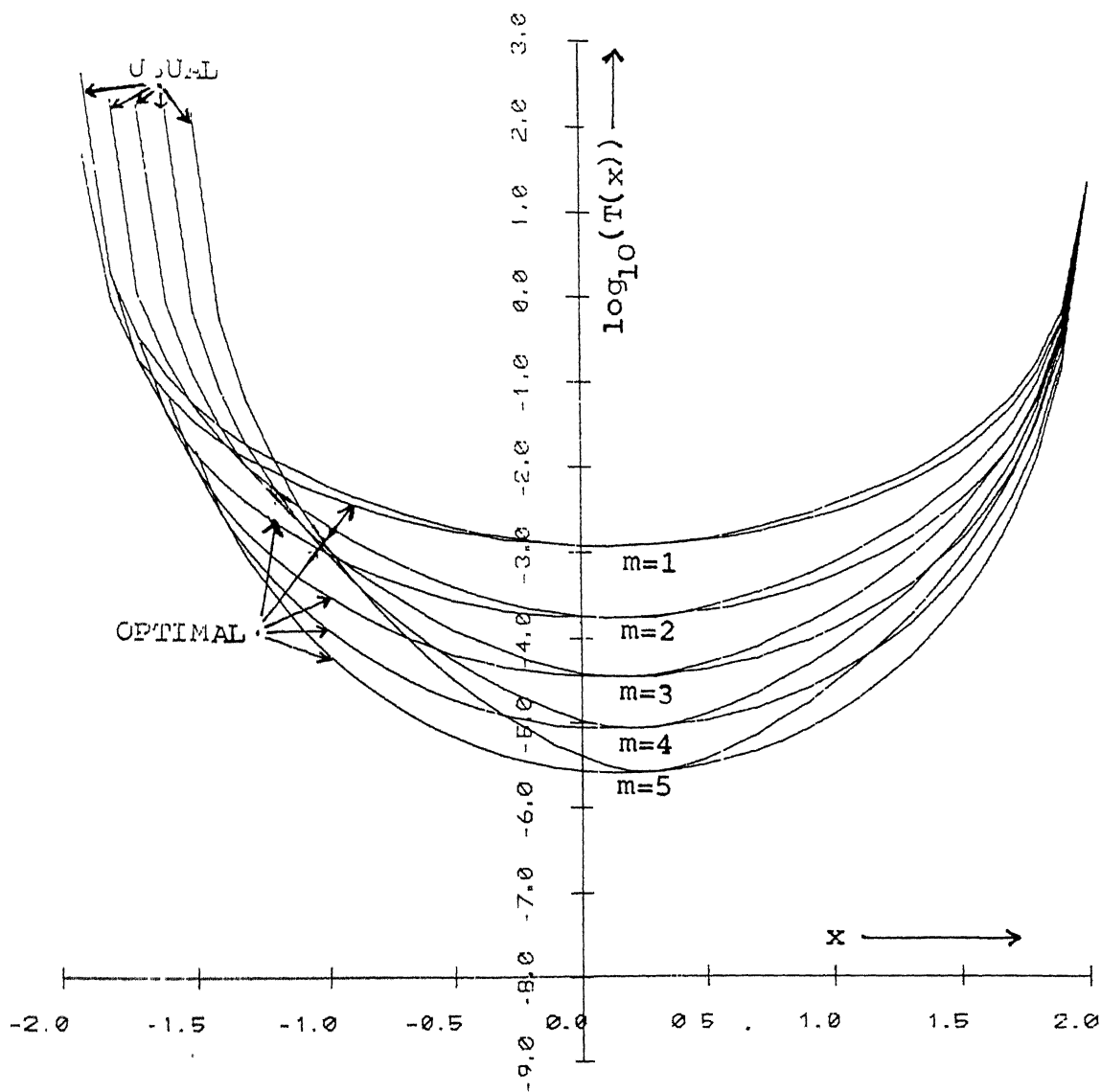


Figure 4.1: Local Truncation Error in Explicit  $L^2(\hat{C}_r)$  -  
 Quadrature Optimal Multistep Methods/  
 Usual Methods ( $r=2.01$ ,  $h=0.1$ )



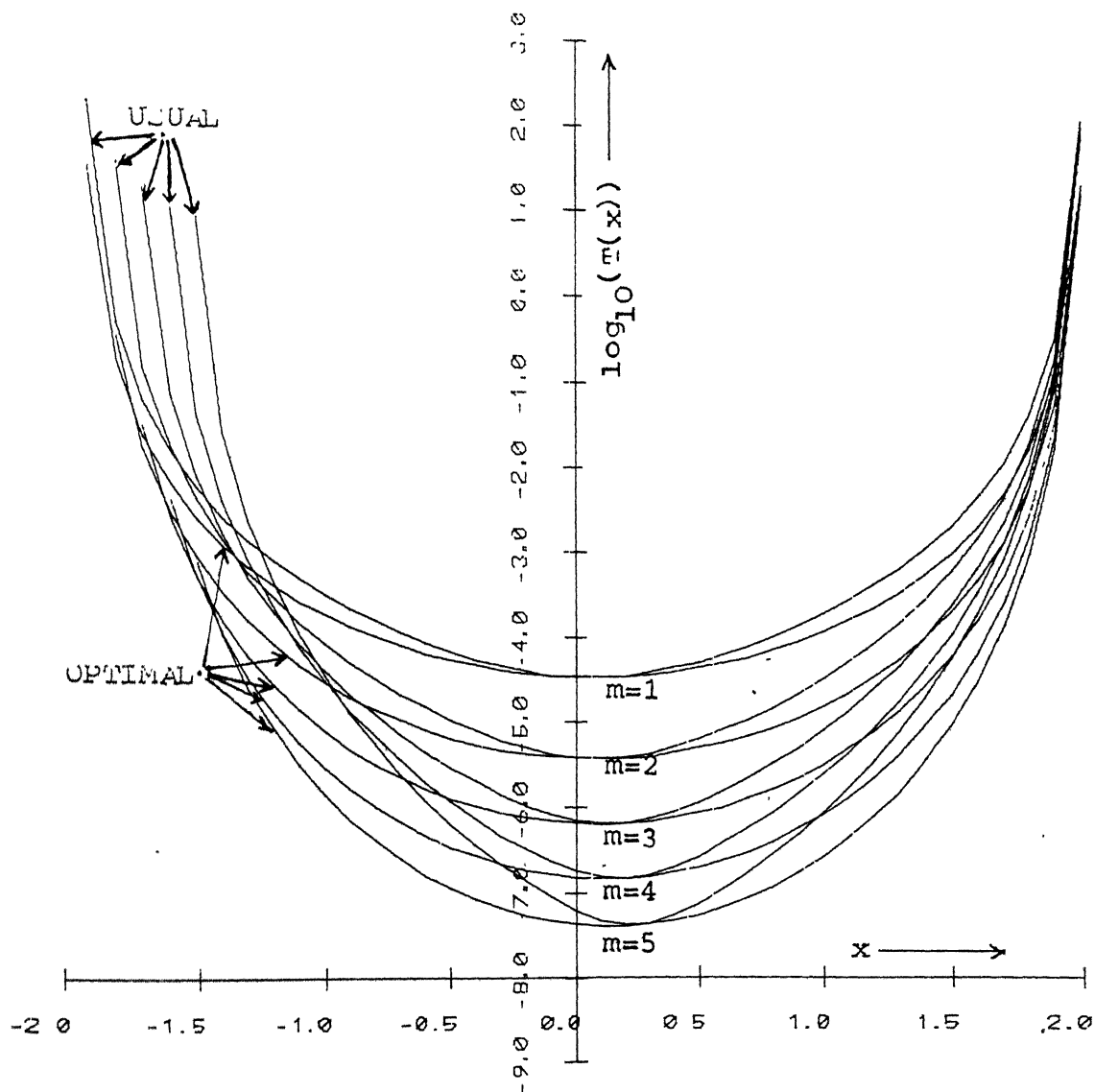


Figure 4.2: Local Truncation Error in Implicit  $L^2(\hat{C}_r^*)$  -  
 Quadrature Optimal Multistep Methods/  
 Usual Methods ( $r=2.01$ ,  $h=0.1$ )



Table 4.10

End point  $(x_N=1.2)$  errors for implicit  $L^2(\hat{C}_r)$  quadrature  
optimal methods

( $r=2.01$ ,  $h=0.1$ )

Eqn. No.	Usual	$\bar{M}$	$\bar{M}^1$	$\bar{M}^2$	Methods $\bar{M}^3$	$\bar{M}^4$	$\bar{M}^5$	$\bar{M}^F$
1	-.82E-04	-.55E-06	-.55E-06	-.10E-05	-.86E-06	-.42E-05	-.34E-05	-.11E-05
2	-.24E-04	.97E-07	.97E-07	-.20E-06	.24E-06	-.13E-05	-.93E-03	-.60E-07
3	-.19E-03	-.18E-05	-.19E-05	-.25E-05	-.30E-05	-.96E-05	-.13E-04	-.30E-05
4	-.69E-04	-.18E-06	-.17E-06	-.51E-06	-.15E-06	-.30E-05	-.11E-05	-.48E-06
5	-.86E-04	-.33E-06	-.37E-06	.10E-05	-.27E-06	.49E-05	-.13E-05	-.71E-06
6	-.32E-04	-.43E-06	-.44E-06	-.53E-06	-.63E-06	-.17E-05	-.28E-05	-.60E-06
7	-.53E-05	-.59E-07	-.61E-07	-.67E-07	-.84E-07	.27E-06	-.47E-06	-.78E-07
8	-.29E-04	-.36E-06	-.38E-06	-.45E-06	-.34E-06	-.14E-05	-.12E-05	-.45E-06
9	-.12E-04	-.86E-07	-.86E-07	-.86E-07	-.61E-07	-.55E-06	-.51E-06	-.82E-07
10	-.67E-03	-.72E-05	.72E-05	.20E-05	.27E-04	-.13E-03	.36E-03	-.94E-05
11	-.39E+00	.28E-01	.31E-01	.16E-01	.34E+00	-.64E+00	.60E+00	.13E+00
12	.39E+00	-.11E-01	-.15E-01	-.32E-02	-.33E+00	.65E+00	-.60E+00	-.12E+00
13	-.18E-06	.93E-07	.10E-06	-.34E-07	.93E-07	-.10E-06	.15E-06	0.0
14	-.12E-06	.75E-07	.82E-07	-.30E-07	.78E-07	-.78E-07	.86E-07	.37E-08
15	-.28E-06	.61E-07	.61E-07	-.32E-07	.88E-07	-.12E-06	.19E-06	.11E-07
16	-.18E-06	.54E-07	.54E-07	-.24E-07	.82E-07	-.95E-07	.14E-06	.15E-07
17	-.84E-09	.58E-10	.73E-10	.17E-09	.60E-09	-.60E-09	.55E-09	.35E-09
18	-.51E-08	.93E-09	.93E-09	.51E-08	.65E-08	-.51E-08	.47E-08	.47E-08
19	-.22E-03	-.80E-05	-.88E-05	-.11E-04	-.12E-04	-.17E-04	-.19E-04	-.15E-04
20	-.46E-04	-.65E-06	-.81E-06	-.14E-05	-.18E-05	-.34E-05	-.42E-05	-.24E-05
21	-.32E-04	-.12E-05	-.14E-05	-.18E-05	-.16E-05	-.26E-05	.15E-05	-.25E-05
22	-.72E-04	-.42E-05	-.47E-05	-.53E-05	-.42E-05	-.58E-05	-.29E-05	-.61E-05
23	.77E-04	-.89E-05	-.97E-05	-.72E-05	-.57E-05	.18E-05	-.28E-05	-.80E-05
24	-.21E-05	-.85E-07	-.18E-06	-.52E-06	-.57E-06	-.71E-06	-.49E-06	-.10E-05

errors are least for  $\tilde{\underline{M}}$  on equations 7, 11, 12, 18, 19, 20, 21 and 24; for  $\tilde{\underline{M}}^1$  on equations 6 and 18, for  $\tilde{\underline{M}}^2$  on equations 10 and 17; for  $\tilde{\underline{M}}^3$  on equations 1, 4, 5 and 8; for  $\tilde{\underline{M}}^4$  on equation 23; for  $\tilde{\underline{M}}^5$  on equations 4 and 22; and for  $\tilde{\underline{M}}^F$  on equations 2, 9, 13, 14, 15 and 16.

## CHAPTER 5

### OPTIMAL MULTISTEP METHODS IN $L^2(\hat{C}_r)$

#### 5.1 Introduction

In this chapter we consider optimal multistep formulae for the Hilbert space  $L^2(\hat{C}_r)$  of functions. On the whole, the multistep formulae of the present chapter have the same advantages over the corresponding quadrature optimal formulae in  $L^2(\hat{C}_r)$  as the formulae of Chapter 3 have over those of Chapter 2. Concerning the relative growth on  $(-r, r)$  of functions to which the formulae are to be applied, a look at the respective interpolatory functions reveals that the formulae of the present chapter admit functions of a higher growth than those of any of the Chapters 2-4. This is, of course, as might have been expected theoretically from the inclusion  $H^2(C_r) \subset L^2(\hat{C}_r)$ .

In this chapter in Section 5.2 we directly verify that the representer of the derivative evaluation functional in  $L^2(\hat{C}_r)$  is the complex conjugate of the derivative of the kernel function of  $L^2(\hat{C}_r)$ . Section 5.3 contains normal equations for constructing optimal multistep formulae in  $L^2(\hat{C}_r)$ , a characterization of the formulae and numerical tables and results obtained for the

same. In Section 5.4,  $L^2(\hat{c}_r)$ -optimal methods interpolatory for polynomials of a certain degree are presented. In Section 5.5 we consider  $L^2(\hat{c}_r)$  optimal methods interpolatory for a set of prefixed functions. In Section 5.6 limiting behaviour of the coefficients of  $L^2(\hat{c}_r)$ -optimal formulae, as  $r \rightarrow \infty$ , is described. In the last section different methods of this chapter have been compared for their numerical performance.

## 5.2 The Representer of Derivative Evaluation Functional

In Chapter 4 we proved that the derivative evaluation functional at a point inside  $c_r$  is a bounded functional  $L^2(\hat{c}_r)$ . In the following theorem we obtain the representer of the same. We recall here the expression for the kernel function of  $L^2(\hat{c}_r)$ :

$$(1) \quad K(z, \bar{t}) = \frac{r^2}{\pi(r^2 - z\bar{t})^2}.$$

Theorem 1: In the space  $L^2(\hat{c}_r)$ , the representer  $\underline{D}(t, \bar{z}_0)$  of the derivative evaluation functional at a point  $z_0$  inside  $c_r$  is given by

$$(2) \quad \underline{D}(t, \bar{z}_0) = \frac{2r^2 t}{\pi(r^2 - t\bar{z}_0)^3}.$$

Proof. Let  $f \in L^2(\hat{c}_r)$ . Then, for a  $z_0$  inside  $c_r$ , we have

$$\begin{aligned}
& \left( f(z), \frac{2r^2 z}{\pi(r^2 - z\bar{z}_0)^3} \right) \\
&= \iint_{D_r} \frac{f(z) 2r^2 \bar{z}}{\pi(r^2 - z\bar{z}_0)^3} dx dy \\
&= \int_{\rho=0}^r \int_{\theta=0}^{2\pi} \frac{f(\rho e^{i\theta}) 2r^2 \rho e^{-i\theta}}{\pi(r^2 - \rho e^{-i\theta} \bar{z}_0)^3} \rho d\rho d\theta \\
&= \int_{\rho=0}^r \left\{ \int_{\theta=0}^{2\pi} \frac{f(\rho e^{i\theta}) 2r^2}{\pi \left( \frac{r^2}{\rho^2} \rho e^{i\theta} - \bar{z}_0 \right)^3} \frac{(\rho e^{i\theta})^2}{\rho^4} \frac{\rho i e^{i\theta} d\theta}{i e^{i\theta}} \right\} d\rho \\
&= \int_{\rho=0}^r \left\{ \int_{C_r} \frac{f(z) z}{\pi i \left( z - \frac{z_0 \rho^2}{r^2} \right)^3} \frac{r^2 2(\rho^2/r^2)^3}{\rho^3} dz \right\} d\rho \\
&= \int_{\rho=0}^r \left[ f(z) z \right]'_{z = \frac{\rho^2}{r^2} z_0} \frac{2\rho^3}{r^4} d\rho,
\end{aligned}$$

by a Cauchy integral formula (for second derivative).

If  $z_0 = 0$ , the last integral equals

$$\int_{\rho=0}^r \left[ f''(0) \cdot 0 + 2 f'(0) \right] \frac{d\rho^3}{r^4} d\rho = f'(0).$$

On the other hand, if  $z_0 \neq 0$ , the integral equals

$$\begin{aligned}
& \int_{z=0}^{z_0} \left[ f(z) z \right]' \frac{z}{z_0} dz \\
&= \frac{1}{z_0^2} \left[ \left\{ z [f(z) z]' \right\} \Big|_{z=0}^{z_0} - \int_{z=0}^{z_0} [f(z) z]' dz \right] \\
&= f'(z_0).
\end{aligned}$$

Thus the proof is complete.

Note that (2) is equivalent to saying that

$$D(t, \bar{z}_0) = \overline{(\partial K(z, \bar{t}) / \partial z)} \Big|_{z=\bar{z}_0}.$$

### 5.3 Optimal Multistep Methods in $L^2(\hat{C}_r)$

The coefficients  $\hat{b}_j$  of an optimal multistep formula

$$(3) \quad Y_{n+1} = \sum_{i=1}^m a_i Y_{n+1-i} + h \sum_{j=\delta_{to}}^m \hat{b}_j f(x_{n+1-j}, Y_{n+1-j}),$$

with  $a_i$ 's chosen according to same known usual method, satisfy the equations

$$(4) \quad \hat{C} \hat{b} = \hat{d}$$

with 
$$\hat{b} = [\hat{b}_{\delta_{to}}, \dots, \hat{b}_m]^T,$$

$$(5) \quad \hat{C}_{ij} = \frac{2r^2}{\pi} \left\{ \frac{(r^2 + 2x_{n+1-j} \bar{x}_{n+1-i})}{(r^2 - x_{n+1-j} \bar{x}_{n+1-i})^4} \right\}$$

and

$$(6) \quad \hat{d}_i = \frac{2r^2}{\pi h} \bar{x}_{n+1-i} \{ (r^2 - x_{n+1} \bar{x}_{n+1-i})^{-3} - \sum_{k=1}^n a_k (r^2 - x_{n+1-k} \bar{x}_{n+1-i})^{-3} \}, \quad i, j = \delta_{to}(1)m.$$

The following theorem characterizes the multistep formula (3).

Theorem 2: The optimal multistep formula (3) is locally interpolatory for functions  $\{x(r^2 - \bar{x}_{n+1-i} x)^{-3}; i=\delta_{to}(1)m\}$ .

Proof. The proof is an easy consequence of (4) or of Theorem 1.4 and (2).



It may be noted that if  $x_{n+1-i} = 0$  for some  $i = \delta_{to}(1)m$  and  $\sum a_i = 1$  then the formula (3) is exact for polynomials of degree one.

We also observe from Theorem 3 that the growth of the interpolatory functions for (3) is according to the third power of  $(r^2 - \bar{x}_{n+1-i}x)^{-1}$ . The same for quadrature optimal  $H^2(c_r)$ , optimal  $H^2(c_r)$  and quadrature optimal  $L^2(\hat{c}_r)$  is according to  $\log(r^2 - \bar{x}_{n+1-i}x)$ ,  $(r^2 - \bar{x}_{n+1-i}x)^{-2}$  and  $(r^2 - \bar{x}_{n+1-i}x)^{-1}$ , respectively. This substantiates the remark made in the first section of this chapter.

The  $L^2(\hat{c}_r)$ -norm of the local truncation error  $\underline{T}_n$  at  $x_{n+1}$  for a general multistep formula

$$y_{n+1} = \sum_{i=n+1-i}^m a_i y_{n+1-i} + h \sum_{j=\delta_{to}}^m b_j f(x_{n+1-j}, y_{n+1-j})$$

is given by

$$\begin{aligned} (7) \quad ||\underline{T}_n||^2 &= \frac{r^2}{\pi} \left[ (r^2 - |x_{n+1}|^2)^{-2} - \sum_{i=1}^m a_i (r^2 - \bar{x}_{n+1}x_{n+1-i})^{-2} \right. \\ &\quad - \sum_{i=1}^m \bar{a}_i \{ (r^2 - x_{n+1}\bar{x}_{n+1-i})^{-2} \\ &\quad - \sum_{j=1}^m a_j (r^2 - x_{n+1-j}\bar{x}_{n+1-i})^{-2} \} - h \sum_{j=\delta_{to}}^m b_j g(x_{n+1-j}) \\ &\quad - h \sum_{k=\delta_{to}}^m \bar{b}_k \overline{g(x_{n+1-k})} \\ &\quad \left. - 2h \sum_{j=\delta_{to}}^m b_j \frac{r^{2+2x_{n+1-j}\bar{x}_{n+1-k}}}{(r^2 - x_{n+1-j}\bar{x}_{n+1-k})^4} \right] , \end{aligned}$$

where

$$(8) \quad g(x) = 2x[(r^2 - \bar{x}_{n+1}x)^{-3} - \sum_{l=1}^m \bar{a}_l (r^2 - \bar{x}_{n+1-l}x)^{-3}].$$

Using the normal equations (4), the norm of the local truncation error  $\hat{T}_n$  for the optimal formula (3) can be simplified as

$$(9) \quad \|\hat{T}_n\|^2 = \frac{r^2}{\pi} [(r^2 - |x_{n+1}|^2)^{-2} - \sum_{i=1}^m a_i (r^2 - \bar{x}_{n+1}x_{n+1-i})^{-2} \\ - \sum_{i=1}^m \bar{a}_i \{(r^2 - x_{n+1}\bar{x}_{n+1-i})^{-2} \\ - \sum_{j=1}^m a_j (r^2 - x_{n+1-j}\bar{x}_{n+1-i})^{-2}\} \\ - h \sum_{j=\delta_{to}}^m \hat{b}_j g(x_{n+1-j})],$$

where  $g(x)$  is as in (8).

Numerically computed results for  $L^2(\hat{C}_r)$ -optimal 5-step methods are presented in Tables 5.1 and 5.1(a)-(d). Table 5.1 displays the coefficients and the error norms for the optimal method. The optimal error norms at the beginning of the table have now reduced further (as compared to Chapters 2-4). The general behaviour of the coefficients however, has been observed to be as in the earlier chapters. As seen from Tables 5.1(a)-(d) the explicit  $L^2(\hat{C}_r)$ -optimal multistep method has been just better

Table 5.1

SITUATION: Y IN 2 (C.F.) ; R = 2.01 H = .10  
MULTI STEP METHOD OF 5 STEPS

X	EUSUAL	OPTIMAL	H X B(1)	H X B(2)	H X B(3)	H X B(4)	H X B(5)
0	0	0	0	0	0	0	0
1	0	0	0	0	0	0	0
2	0	0	0	0	0	0	0
3	0	0	0	0	0	0	0
4	0	0	0	0	0	0	0
5	0	0	0	0	0	0	0
6	0	0	0	0	0	0	0
7	0	0	0	0	0	0	0
8	0	0	0	0	0	0	0
9	0	0	0	0	0	0	0
10	0	0	0	0	0	0	0
11	0	0	0	0	0	0	0
12	0	0	0	0	0	0	0
13	0	0	0	0	0	0	0
14	0	0	0	0	0	0	0
15	0	0	0	0	0	0	0
16	0	0	0	0	0	0	0
17	0	0	0	0	0	0	0
18	0	0	0	0	0	0	0
19	0	0	0	0	0	0	0
20	0	0	0	0	0	0	0
21	0	0	0	0	0	0	0
22	0	0	0	0	0	0	0
23	0	0	0	0	0	0	0
24	0	0	0	0	0	0	0
25	0	0	0	0	0	0	0
26	0	0	0	0	0	0	0
27	0	0	0	0	0	0	0
28	0	0	0	0	0	0	0
29	0	0	0	0	0	0	0
30	0	0	0	0	0	0	0
31	0	0	0	0	0	0	0
32	0	0	0	0	0	0	0
33	0	0	0	0	0	0	0
34	0	0	0	0	0	0	0
35	0	0	0	0	0	0	0
36	0	0	0	0	0	0	0
37	0	0	0	0	0	0	0
38	0	0	0	0	0	0	0
39	0	0	0	0	0	0	0
40	0	0	0	0	0	0	0
41	0	0	0	0	0	0	0
42	0	0	0	0	0	0	0
43	0	0	0	0	0	0	0
44	0	0	0	0	0	0	0
45	0	0	0	0	0	0	0
46	0	0	0	0	0	0	0
47	0	0	0	0	0	0	0
48	0	0	0	0	0	0	0
49	0	0	0	0	0	0	0
50	0	0	0	0	0	0	0
51	0	0	0	0	0	0	0
52	0	0	0	0	0	0	0
53	0	0	0	0	0	0	0
54	0	0	0	0	0	0	0
55	0	0	0	0	0	0	0
56	0	0	0	0	0	0	0
57	0	0	0	0	0	0	0
58	0	0	0	0	0	0	0
59	0	0	0	0	0	0	0
60	0	0	0	0	0	0	0
61	0	0	0	0	0	0	0
62	0	0	0	0	0	0	0
63	0	0	0	0	0	0	0
64	0	0	0	0	0	0	0
65	0	0	0	0	0	0	0
66	0	0	0	0	0	0	0
67	0	0	0	0	0	0	0
68	0	0	0	0	0	0	0
69	0	0	0	0	0	0	0
70	0	0	0	0	0	0	0
71	0	0	0	0	0	0	0
72	0	0	0	0	0	0	0
73	0	0	0	0	0	0	0
74	0	0	0	0	0	0	0
75	0	0	0	0	0	0	0
76	0	0	0	0	0	0	0
77	0	0	0	0	0	0	0
78	0	0	0	0	0	0	0
79	0	0	0	0	0	0	0
80	0	0	0	0	0	0	0
81	0	0	0	0	0	0	0
82	0	0	0	0	0	0	0
83	0	0	0	0	0	0	0
84	0	0	0	0	0	0	0
85	0	0	0	0	0	0	0
86	0	0	0	0	0	0	0
87	0	0	0	0	0	0	0
88	0	0	0	0	0	0	0
89	0	0	0	0	0	0	0
90	0	0	0	0	0	0	0
91	0	0	0	0	0	0	0
92	0	0	0	0	0	0	0
93	0	0	0	0	0	0	0
94	0	0	0	0	0	0	0
95	0	0	0	0	0	0	0
96	0	0	0	0	0	0	0
97	0	0	0	0	0	0	0
98	0	0	0	0	0	0	0
99	0	0	0	0	0	0	0
100	0	0	0	0	0	0	0

Table 5.1(a)

[illegible]

Table 5.1(b)

[illegible]

Table 5.1(c)

[illegible]



Table 5.1(d)

[illegible]

on equations 13, 16 and 24; one decimal place better on equations 2, 8, 10, 12, 15, 17, 18, 19, 20, 21, 22 and 23; two decimal places better on equations 1, 3, 4, 5, 6 and 11; and three decimal places better on equations 7 and 9, in comparison to the 5-step Adams-Bashforth method. As compared to 5-step Adams-Moulton method, the implicit  $L_2(\hat{C}_r)$ -optimal 5-step method has been just better on equations 16, 15, 17, 18 and 24; one decimal place better on equations 5, 10, 11, 12, 19, 20, 21, 22 and 23; two decimal places better on equations 1, 2, 4 and 7; and three decimal places better on equations 3, 6, 8 and 9.

#### 5.4 Optimal Multistep Methods in $L^2(\hat{C}_r)$ Interpolatory for Polynomials

As was done in Section 3.6 for the space  $H^2(C_r)$ , we consider here, for the space  $L^2(\hat{C}_r)$ , the optimal multistep formulae interpolatory for polynomials corresponding to the special situation of equispaced points on a line within  $C_r$ . Let the distance between the consecutive points be  $h$ . The coefficients  $\hat{\gamma}^P$  of an  $L^2(\hat{C}_r)$ -optimal multistep formula

$$(10) \quad y_{n+1} - \sum_{i=1}^m a_i y_{n+1-i} - h \sum_{j=0}^{p-1} \gamma_j^u \nabla^j f(x_{n+\delta_{t1}}, y_{n+\delta_{t1}}) \\ = h \sum_{j=p}^{m-\delta_{t0}} \hat{\gamma}_j^P \nabla^j f(x_{n+\delta_{t1}}, y_{n+\delta_{t1}}),$$

interpolatory for polynomials of degree  $p < m + \delta_{t1}$ , with



prefixed  $a_i$ 's such that  $\sum a_i = 1$  and with  $\gamma_j^u$ 's as for the corresponding usual formulae, are to satisfy the normal equations

$$(11) \quad \underline{\hat{C}}^P \underline{\hat{\gamma}}^P = \underline{\hat{d}}^P$$

where

$$(12) \quad \underline{\hat{\gamma}}^P = (\hat{\gamma}_p^P, \dots, \hat{\gamma}_{m-\delta_{t0}}^P)^T,$$

$$(13) \quad \hat{C}_{ij}^P = \frac{2r^2}{\pi} \sum_{k=0}^j \sum_{l=0}^i (-1)^{l+k} \binom{i}{l} \binom{j}{k} \frac{(r^{2+2x_{n+\delta_{t1}}-k} \bar{x}_{n+\delta_{t1}-l})}{(r^{2-x_{n+\delta_{t1}}-k} \bar{x}_{n+\delta_{t1}-l})^4},$$

$$(14) \quad \hat{d}_i^P = \frac{2r^2}{\pi h} \left[ \sum_{l=0}^i (-1)^l \binom{i}{l} \bar{x}_{n+\delta_{t1}-l} \{ (r^{2-x_{n+1}} \bar{x}_{n+\delta_{t1}-l})^{-3} - \sum_{q=1}^m a_q (r^{2-x_{n+1}-q} \bar{x}_{n+\delta_{t1}-l})^{-3} \} \right]$$

$$- \frac{2r^2}{\pi} \sum_{q=0}^{p-1} \gamma_q^u \{ \sum_{k=0}^q \sum_{l=0}^i (-1)^{l+k} \binom{i}{l} \binom{q}{k} \cdot$$

$$\cdot \frac{r^{2+2x_{n+\delta_{t1}}-k} \bar{x}_{n+\delta_{t1}-l}}{(r^{2-x_{n+\delta_{t1}}-k} \bar{x}_{n+\delta_{t1}-l})^3 \},$$

$$i, j = p(1)m - \delta_{t0}.$$

The above described method is characterized as follows:

Theorem 3: The  $L^2(\hat{C}_r)$ -optimal multistep formula (10) interpolatory for polynomials of degree  $p < m + \delta_{t1}$  is

characterized by being interpolatory for functions

$$\underline{h}_j(x) = \sum_{k=0}^j (-1)^k \binom{j}{k} \frac{x}{(r^2 - \bar{x}_{n+\delta_{t1}} - kx)^3}, \quad j = p(1)m - \delta_{t0}.$$

Proof: The proof is an easy consequence of (2) and (11).

To compute  $\hat{\underline{b}}_j^P$ ,  $j = \delta_{t0}(1)m$ , in the alternate representation

$$(15) \quad Y_{n+1} = \sum_{i=1}^m a_i Y_{n+1-i} + h \sum_{j=\delta_{t0}}^m \hat{\underline{b}}_j^P f(x_{n+1-j}, Y_{n+1-j})$$

of (10), we use the relations

$$(16) \quad \hat{\underline{b}}_{l+\delta_{t0}}^P = (-1)^l \sum_{j=1}^{m-\delta_{t0}} \binom{j}{l} \gamma_j^*, \quad l = 0(1)m - \delta_{t0},$$

where

$$(17) \quad \gamma_j^* = \begin{cases} \gamma_j^u & , 0 \leq j \leq p-1 \\ \hat{\gamma}_j^P & , p \leq j \leq m - \delta_{t0} \end{cases}.$$

It is important to note that  $\gamma_j^u$ 's are different in the explicit and the implicit situations.

In Tables 5.2-5.6 we present the coefficients  $\hat{\underline{b}}_j^P$  and the error norms of the  $L^2(\hat{C}_r)$ -optimal 5-step methods interpolatory for polynomials of degree  $p = 1(1)5$ . We observe that the general behaviour of the error norms and the coefficients is the same as in the case of Chapters 2-4. A summary of numerical results obtained by using these coefficients on the set of twenty four differential equations is as follows:

[illegible]





Table 5.5

SITUATION: Y IN L<sup>2</sup>(C I) R= 2.01 H= 10  
MULTI STEP METHOD OF 5 STEPS INTERPOLATORY UPTO 4 DEGREE POLYNOMIALS

X	EUSUAL	EOPIMAL	H X B(1)	H X B(2)	H X B(3)	H X B(4)	H X B(5)
0	0	0	0	0	0	0	0
1	0	0	0	0	0	0	0
2	0	0	0	0	0	0	0
3	0	0	0	0	0	0	0
4	0	0	0	0	0	0	0
5	0	0	0	0	0	0	0
6	0	0	0	0	0	0	0
7	0	0	0	0	0	0	0
8	0	0	0	0	0	0	0
9	0	0	0	0	0	0	0
10	0	0	0	0	0	0	0
11	0	0	0	0	0	0	0
12	0	0	0	0	0	0	0
13	0	0	0	0	0	0	0
14	0	0	0	0	0	0	0
15	0	0	0	0	0	0	0
16	0	0	0	0	0	0	0
17	0	0	0	0	0	0	0
18	0	0	0	0	0	0	0
19	0	0	0	0	0	0	0
20	0	0	0	0	0	0	0
21	0	0	0	0	0	0	0
22	0	0	0	0	0	0	0
23	0	0	0	0	0	0	0
24	0	0	0	0	0	0	0
25	0	0	0	0	0	0	0
26	0	0	0	0	0	0	0
27	0	0	0	0	0	0	0
28	0	0	0	0	0	0	0
29	0	0	0	0	0	0	0
30	0	0	0	0	0	0	0
31	0	0	0	0	0	0	0
32	0	0	0	0	0	0	0
33	0	0	0	0	0	0	0
34	0	0	0	0	0	0	0
35	0	0	0	0	0	0	0
36	0	0	0	0	0	0	0
37	0	0	0	0	0	0	0
38	0	0	0	0	0	0	0
39	0	0	0	0	0	0	0
40	0	0	0	0	0	0	0
41	0	0	0	0	0	0	0
42	0	0	0	0	0	0	0
43	0	0	0	0	0	0	0
44	0	0	0	0	0	0	0
45	0	0	0	0	0	0	0
46	0	0	0	0	0	0	0
47	0	0	0	0	0	0	0
48	0	0	0	0	0	0	0
49	0	0	0	0	0	0	0
50	0	0	0	0	0	0	0
51	0	0	0	0	0	0	0
52	0	0	0	0	0	0	0
53	0	0	0	0	0	0	0
54	0	0	0	0	0	0	0
55	0	0	0	0	0	0	0
56	0	0	0	0	0	0	0
57	0	0	0	0	0	0	0
58	0	0	0	0	0	0	0
59	0	0	0	0	0	0	0
60	0	0	0	0	0	0	0
61	0	0	0	0	0	0	0
62	0	0	0	0	0	0	0
63	0	0	0	0	0	0	0
64	0	0	0	0	0	0	0
65	0	0	0	0	0	0	0
66	0	0	0	0	0	0	0
67	0	0	0	0	0	0	0
68	0	0	0	0	0	0	0
69	0	0	0	0	0	0	0
70	0	0	0	0	0	0	0
71	0	0	0	0	0	0	0
72	0	0	0	0	0	0	0
73	0	0	0	0	0	0	0
74	0	0	0	0	0	0	0
75	0	0	0	0	0	0	0
76	0	0	0	0	0	0	0
77	0	0	0	0	0	0	0
78	0	0	0	0	0	0	0
79	0	0	0	0	0	0	0
80	0	0	0	0	0	0	0
81	0	0	0	0	0	0	0
82	0	0	0	0	0	0	0
83	0	0	0	0	0	0	0
84	0	0	0	0	0	0	0
85	0	0	0	0	0	0	0
86	0	0	0	0	0	0	0
87	0	0	0	0	0	0	0
88	0	0	0	0	0	0	0
89	0	0	0	0	0	0	0
90	0	0	0	0	0	0	0
91	0	0	0	0	0	0	0
92	0	0	0	0	0	0	0
93	0	0	0	0	0	0	0
94	0	0	0	0	0	0	0
95	0	0	0	0	0	0	0
96	0	0	0	0	0	0	0
97	0	0	0	0	0	0	0
98	0	0	0	0	0	0	0
99	0	0	0	0	0	0	0
100	0	0	0	0	0	0	0



As compared to a 5-step Adams-Bashforth method, the explicit  $L^2(\hat{C}_r)$ -optimal method with  $p=1$  has performed just better on equations 17,18 and 24; one decimal place better on equations 2,6,8,10,11,12,19,20,22 and 23; two decimal places better on equations 1,3,4,5,9 and 21; and three decimal places better on equation 7. On equations 13,14 and 16, however, the optimal explicit method has been just worse than the usual method and comparable on equation 15. In comparison to 5-step Adams Moulton method the implicit  $L^2(\hat{C}_r^*)$ -optimal method with  $p=1$  has been comparable on equations 14,15 and 16; just better on equations 13,17,18 and 23; one decimal place better on equations 5,10,12,19,20,21,22 and 24; and two decimal places better on equations 1,2,3,4,6,7,8,9 and 11.

The optimal explicit method with  $p=2$  has performed just better on equations 17,18 and 24; one decimal place better on equations 2,8,15,16,19,20,21,22 and 23; two decimal places better on equations 1,3,4,5,6,9 and 10; and three decimal places better on equation 7. The implicit method with  $p=2$  has been just better on equations 15,16,17, 18 and 24; one decimal place better on equations 5,10,19,20, 21,22 and 23; and two decimal places better on equations 1,2,3,4,6,7,8 and 9. Both the optimal methods have been comparable on the remaining equations 11,12,13 and 14.



The optimal explicit method with  $p=3$  has performed just better on equations 15 and 24; one decimal place better on equations 1,2,3,5,6,8,9,10,19,22 and 23; and two decimal places better on equations 4,7,20 and 21. The optimal implicit method has been just better on equations 15 and 24; one decimal place better on equations 1,2,4,5,10,19,20,21,22 and 23; two decimal places better on equations 3,7,8 and 9; and three decimal places better on equation 6. The implicit and explicit optimal methods, both, have been comparable on equations 11 and 16; and just worse on equations 12,13,14,17 and 18 as compared to the usual methods.

The optimal explicit method with  $p=4$  has performed just better on equations 2,10 and 24; one decimal place better on equations 1,3,4,5,6,8,9,19,20,21,22 and 23; and two decimal places better on equation 7. The optimal implicit method has been just better on equations 10 and 24; one decimal place better on equations 1,2,3,4,5,6,7,8,19,20,21,22 and 23; and two decimal places better on equation 9. Both the implicit and explicit optimal methods have been comparable on equations 13,14,15,16 and 17; and just worse on equations 11,12 and 18.

The implicit optimal method with  $p=5$  was found just better on equations 10,15,17; one decimal place better on equations 1,2,4,5,8,19,20,21,22,23 and 24; and two decimal

places better on equations 3,6,7 and 9. This method has been comparable on equations 13,14 and 16; and just worse on equations 11,12 and 18.

### 5.5 Optimal Multistep Methods in $L^2(\hat{C}_r)$ Interpolatory for a Set of Preassigned Functions

The coefficients  $\hat{\underline{b}}_j^F$  of an optimal multistep formula

$$(18) \quad Y_{n+1} = \sum_{i=1}^m a_i Y_{n+1-i} + h \sum_{j=\delta_{to}}^m \hat{\underline{b}}_j^F f(x_{n+1-j}, Y_{n+1-j})$$

in  $L^2(\hat{C}_r)$ , interpolatory for functions  $\{\varphi_1, \dots, \varphi_p\}$ , can be obtained by solving linear equations

$$(19) \quad \begin{bmatrix} \hat{\underline{C}} & F^* \\ F & 0 \end{bmatrix} \begin{bmatrix} \hat{\underline{b}}^F \\ \lambda \end{bmatrix} = \begin{bmatrix} \hat{\underline{d}} \\ e \end{bmatrix},$$

where  $\hat{\underline{C}}, \hat{\underline{d}}$  are as in (4),  $\lambda = [\lambda_1, \dots, \lambda_p]^T$ ,

$$\hat{\underline{b}}^F = [\hat{\underline{b}}_{\delta_{to}}^F, \dots, \hat{\underline{b}}_m^F]^T,$$

$$F = [\varphi_i(x_{n+1-j})]_{i=1, j=\delta_{to}}^{p,m},$$

$$e_i = \varphi_i(x_{n+1}) - \sum_{j=1}^m a_j \varphi_i(x_{n+1-j}), \quad i=1(1)p,$$

and 0 is a  $p \times p$  null matrix.

The above method is characterized by

Theorem 4: An optimal multistep method in  $L^2(\hat{C}_r)$  interpolatory for linearly independent functions  $\{\varphi_1, \dots, \varphi_p\}$  is locally interpolatory for functions



$$\underline{h}_k(x) = \frac{x}{(r^2 - \bar{x}_{n+1-k}x)^3} + \sum_{i=m-p+1}^m \bar{g}_i^{-m+p, k+1-\delta_{t0}} \frac{x}{(r^2 - \bar{x}_{n+1-i}x)},$$

$$k = \delta_{t0}(1)m-p,$$

where

$$G = [g_{iq}]_{\substack{i=1(1)p \\ q=1(1)m-p+\delta_{t1}}} = P^{-1}E,$$

in which  $P = [\varphi'_i(x_{n+1-j})]_{\substack{i=1(1)p \\ j=m+1-p(1)m}}$  is assumed non-

singular and  $E = [\varphi'_i(x_{n+1-j})]_{\substack{i=1(1)p \\ j=\delta_{t0}(1)m-p}}$

Proof: The proof is immediate from Theorem 1.8, using (2).

In Table 5.7 we present the error norms and coefficients of  $L^2(c_r)$ -optimal 5-step methods interpolatory for functions  $\varphi_1(x) = \exp(1.6x)$  and  $\varphi_2(x) = \exp(-1.6x)$ . The general behaviour of the coefficients and the error norms in the present case is found to be the same as is the case of Chapters 2 to 4. The performance of these methods as compared to usual 5-step methods on the twenty four differential equations has been as follows:

The explicit optimal method interpolatory for  $\exp(1.6x)$  and  $\exp(-1.6x)$  has performed just better on equations 16, 17, 18 and 24; one decimal place better on equations 15, 19, 20, 21, 22 and 23; two decimal places better on equations 1, 2, 3, 4, 5, 6, 8, 9, 10; and three decimal places better on equation 7. In the implicit case the method has been just better on equations 17, 18, 23 and 24; one

decimal place better on equations 5,15,16,19,20,21 and 22;  
 two decimal places better on equations 2,3, 6,7,8,9,10;  
 and three decimal places better on equations 1 and 4.  
 The explicit and implicit methods, both, have worked comparably on the remaining equations 11,12,13 and 14.

### 5.6 Limiting Behaviour of coefficients as $r \rightarrow \infty$

In this section we describe the limiting behaviour of the coefficients of optimal and various interpolatory optimal multistep formulae in the space  $L^2(\hat{C}_r)$ . Since the remarks made at the beginning of Section 4.6, concerning the proofs of various results, remain applicable in the present case as well, only the statements of the results are given.

Theorem 5: Let

$$(20) \quad Y_{n+1} = \sum_{i=1}^m a_i Y_{n+1-i} + h \sum_{j=\delta_{t_0}}^m b_j^F f(x_{n+1-j}, Y_{n+1-j})$$

be a multistep formula interpolatory for functions  $\{\varphi_{\delta_{t_0}}, \dots, \varphi_m\}$  and let the matrix  $[\varphi_i^F(x_{n+1-j})]_{i,j=\delta_{t_0}}^m$  be non-singular. Let

$$(21) \quad Y_{n+1} = \sum_{i=1}^m a_i Y_{n+1-i} + h \sum_{j=\delta_{t_0}}^m \hat{b}_{jr}^F f(x_{n+1-j}, Y_{n+1-j})$$

be an optimal multistep formula in  $L^2(\hat{C}_r)$  interpolatory for functions  $\{\varphi_{\delta_{t_0}}, \dots, \varphi_{p-1+\delta_{t_0}}\}$ ,  $0 \leq p \leq m - \delta_{t_0}$

( $p=0$  being the non-interpolatory case). If the local truncation error functional  $\hat{T}_{nr}^F$  for (20) satisfies

$$\lim_{r \rightarrow \infty} \hat{T}_{nr}^F(\varphi_j) = 0, \quad j = p + \delta_{to}(1)m,$$

then

$$\lim_{r \rightarrow \infty} \hat{b}_{jr}^F = b_j^F, \quad j = \delta_{to}(1)m.$$

Theorem 6. Let  $a_i, i=1(1)m$  be given constants satisfying  $\sum a_i = 1$ . Then the  $L^2(\hat{C}_r)$ -coefficients  $\hat{b}_{jr}$  of an optimal multistep formula

$$(22) \quad y_{n+1} = \sum_{i=1}^m a_i y_{n+1-i} + h \sum_{j=\delta_{to}}^m \hat{b}_{jr} f(x_{n+1-j}, y_{n+1-j})$$

approach the coefficients of the corresponding usual formula as  $r \rightarrow \infty$ .

Theorem 7: Let  $a_i, i=1(1)m$ , be given constants such that  $\sum a_i = 1$ . Then the  $L^2(\hat{C}_r)$ -coefficients  $b_{jr}^P$  of an optimal multistep formula

$$(23) \quad y_{n+1} = \sum_{i=1}^m a_i y_{n+1-i} + h \sum_{j=\delta_{to}}^m \hat{b}_{jr}^P f(x_{n+1-j}, y_{n+1-j}),$$

interpolatory for polynomials of degree  $p < m + \delta_{t1}$ , approach the coefficients of the corresponding usual formula as  $r \rightarrow \infty$ .

Theorem 8: Let  $a_i, i=1(1)m$ , be given constants such that  $\sum a_i = 1$ . Let the matrix

$$M = \begin{bmatrix} \varphi'_1(x_{n+\delta_{t1}}) & \dots & \varphi'_1(x_{n+1-m}) \\ \vdots & & \vdots \\ \varphi'_p(x_{n+\delta_{t1}}) & \dots & \varphi'_p(x_{n+1-m}) \\ 1 & \dots & 1 \\ x_{n+\delta_{t1}} & \dots & x_{n+1-m} \\ \vdots & & \vdots \\ m-p-\delta_{t0} & \dots & m-p-\delta_{t0} \\ x_{n+\delta_{t1}} & \dots & x_{n+1-m} \end{bmatrix}$$

be non-singular. Then the  $L^2(\hat{C}_r)$ -coefficients  $\hat{b}_{jr}^F$  of an optimal multistep formula

$$(24) \quad y_{n+1} = \sum_{i=1}^m a_i y_{n+1-i} + h \sum_{j=\delta_{t0}}^m \hat{b}_{jr}^F f(x_{n+1-j}, y_{n+1-j}),$$

interpolatory for the functions  $\{\varphi_1, \dots, \varphi_p\}$ ,  $p < m + \delta_{t1}$ , approach the coefficients  $b_j^F$  of the unique multistep formula

$$(25) \quad y_{n+1} = \sum_{i=1}^m a_i y_{n+1-i} + h \sum_{j=\delta_{t0}}^m b_j^F f(x_{n+1-j}, y_{n+1-j}),$$

interpolatory for functions  $\{\varphi_1, \dots, \varphi_p, x, x^2, \dots, x^{m-p+\delta_{t1}}\}$ .

### 5.7 A Comparison of Different Methods

In Table 5.8, the end point ( $x_N=1.2$ ) errors for the set of twenty four differential equations for 1 to 4 step explicit and implicit  $L^2(\hat{C}_r)$ -optimal methods, along

Table 5.8

SITUATION: Y IN  $L(C, F)$  ; R= 2.01 H= .10  
 ERRORS AT END POINT FOR EXPLICIT METHODS

Eq.No.	M	1		2		3		4	
		USUAL	OPTIMAL	USUAL	OPTIMAL	USUAL	OPTIMAL	USUAL	OPTIMAL
1.		-0.41E-01	-0.18E-01	0.25E-02	0.91E-04	-0.30E-02	-0.65E-03	0.17E-02	-0.16E-04
2.		-0.32E-01	-0.13E-01	0.16E-02	0.55E-04	-0.17E-02	-0.45E-03	0.75E-03	-0.20E-04
3.		-0.50E-01	-0.23E-01	0.43E-02	0.12E-03	-0.54E-02	-0.99E-03	0.36E-02	-0.39E-05
4.		-0.39E-01	-0.19E-01	0.28E-02	0.18E-04	-0.33E-02	-0.66E-03	0.11E-02	-0.22E-04
5.		-0.12E+00	-0.44E-01	-0.46E-02	-0.62E-03	-0.50E-02	-0.16E-02	-0.22E-02	-0.60E-04
6.		-0.44E-02	-0.24E-02	0.57E-03	-0.30E-04	-0.69E-03	-0.80E-04	0.55E-03	-0.29E-05
7.		-0.50E-03	-0.31E-03	0.96E-03	-0.54E-05	-0.50E-02	-0.93E-05	0.88E-04	-0.16E-05
8.		-0.81E-02	-0.42E-02	0.84E-03	-0.10E-03	-0.94E-03	-0.11E-03	0.59E-03	-0.13E-04
9.		-0.20E-02	-0.12E-02	0.34E-03	-0.13E-04	-0.22E-02	-0.26E-04	0.22E-03	-0.47E-05
10.		-0.17E+01	-0.11E+01	0.17E+00	-0.13E-01	-0.22E-01	-0.36E+01	0.98E+02	-0.15E+02
11.		-0.13E+04	-0.34E+03	0.76E+03	-0.46E+02	-0.22E-01	-0.98E+01	0.98E+02	-0.10E+01
12.		0.13E+04	0.35E+03	-0.17E+03	0.37E+02	-0.22E-01	-0.62E+01	-0.99E+02	-0.69E+00
13.		-0.99E-02	-0.30E-02	0.18E-03	0.73E-04	-0.17E-03	-0.12E-03	0.22E-04	-0.49E-05
14.		-0.85E-02	-0.25E-02	0.14E-03	0.71E-04	-0.13E-03	-0.10E-03	0.19E-04	-0.41E-05
15.		-0.80E-02	-0.27E-02	0.20E-03	0.30E-04	-0.20E-03	-0.97E-04	0.33E-04	-0.46E-05
16.		-0.69E-02	-0.23E-02	0.16E-03	0.32E-04	-0.15E-03	-0.83E-04	0.22E-04	-0.39E-05
17.		-0.67E-05	-0.39E-05	0.82E-06	-0.24E-06	-0.73E-06	-0.26E-07	0.81E-06	-0.18E-07
18.		-0.66E-04	-0.38E-04	0.79E-05	-0.24E-05	-0.69E-06	-0.24E-06	0.81E-06	-0.19E-06
19.		0.63E-01	-0.21E-01	0.53E-02	-0.52E-02	-0.71E-02	-0.59E-03	0.40E-02	-0.17E-02
20.		-0.60E-02	-0.32E-01	0.54E-03	-0.84E-03	-0.63E-03	-0.27E-03	0.77E-03	-0.37E-03
21.		-0.57E-02	-0.33E-01	0.72E-03	-0.11E-02	-0.74E-03	-0.16E-03	0.61E-03	-0.36E-03
22.		-0.22E-01	-0.76E-01	0.28E-02	-0.13E-02	-0.34E-02	-0.31E-03	0.19E-02	-0.75E-03
23.		0.22E+00	-0.77E-01	-0.36E-02	-0.75E-02	0.37E-02	-0.38E-02	-0.20E-02	-0.11E-02
24.		0.97E-04	-0.59E-02	-0.65E-04	-0.52E-03	0.77E-04	-0.12E-03	0.52E-04	-0.22E-03

ERRORS AT END POINT FOR IMPLICIT METHODS

Eq.No.	M	1		2		3		4	
		USUAL	OPTIMAL	USUAL	OPTIMAL	USUAL	OPTIMAL	USUAL	OPTIMAL
1.		-0.19E-03	-0.31E-04	0.27E-03	0.78E-04	-0.58E-04	0.92E-06	0.65E-04	0.44E-05
2.		-0.12E-03	-0.18E-04	0.16E-03	0.55E-04	-0.28E-04	0.13E-05	0.27E-04	0.30E-05
3.		-0.31E-03	-0.53E-04	0.47E-03	0.12E-03	-0.12E-03	-0.30E-06	0.14E-03	0.65E-05
4.		-0.20E-03	-0.38E-04	0.30E-03	0.78E-04	-0.32E-04	-0.10E-05	0.68E-04	0.39E-05
5.		-0.36E-03	-0.82E-04	-0.47E-03	-0.20E-03	-0.10E-04	-0.53E-05	-0.82E-04	-0.12E-06
6.		-0.45E-04	-0.51E-05	0.58E-04	0.89E-05	-0.17E-04	-0.11E-07	0.21E-04	0.48E-06
7.		-0.79E-05	-0.51E-06	0.94E-05	0.86E-06	-0.28E-05	-0.14E-06	0.34E-05	0.57E-07
8.		-0.68E-04	-0.28E-05	0.84E-04	0.12E-04	-0.79E-04	-0.49E-06	0.22E-04	0.48E-06
9.		-0.28E-04	-0.28E-06	0.33E-04	0.22E-05	-0.76E-05	-0.45E-06	0.80E-05	0.10E-06
10.		-0.11E+01	-0.40E-03	0.21E-01	0.41E-02	-0.25E-02	-0.64E-04	0.20E-02	0.15E-03
11.		0.18E+03	-0.53E+01	0.28E+02	0.14E-01	0.60E+01	-0.16E+00	0.15E+01	-0.53E-01
12.		0.18E+03	-0.25E+01	-0.28E+02	0.53E+00	0.60E+01	-0.34E+00	-0.15E+01	0.11E+00
13.		-0.15E-04	-0.66E-05	0.18E-04	0.15E-04	-0.10E-05	0.54E-06	0.69E-06	0.10E-05
14.		-0.12E-04	-0.62E-05	0.14E-04	0.13E-04	-0.68E-06	0.49E-06	0.45E-06	0.89E-06
15.		-0.16E-04	-0.36E-05	0.20E-04	0.12E-04	-0.14E-05	0.41E-06	0.97E-06	0.74E-06
16.		-0.13E-04	-0.34E-05	0.16E-04	0.10E-04	-0.96E-06	0.36E-06	0.68E-06	0.65E-06
17.		-0.73E-07	0.14E-07	0.76E-07	-0.16E-08	-0.46E-08	-0.17E-08	0.30E-08	-0.23E-09
18.		-0.71E-06	0.14E-06	0.73E-06	-0.19E-07	-0.36E-07	-0.18E-07	0.25E-07	-0.14E-08
19.		-0.28E-03	0.42E-03	0.66E-03	-0.47E-04	-0.13E-03	0.88E-04	0.10E-03	-0.27E-04
20.		-0.63E-04	0.94E-04	0.41E-04	0.41E-04	-0.25E-04	0.20E-04	0.30E-04	-0.27E-05
21.		-0.79E-04	0.12E-03	0.57E-04	0.23E-04	-0.23E-04	0.19E-04	0.26E-04	-0.37E-04
22.		-0.17E-03	0.25E-03	0.32E-03	-0.36E-04	-0.55E-04	0.39E-04	0.60E-04	-0.13E-04
23.		0.32E-03	0.71E-03	-0.34E-03	-0.49E-03	-0.72E-03	0.49E-04	-0.74E-04	-0.47E-04
24.		0.46E-06	0.66E-04	-0.11E-04	-0.19E-04	-0.19E-05	0.12E-04	0.14E-05	-0.18E-05



with those for the usual methods, are presented. We observe that the optimal methods have performed better in all the cases except in the case of equation 24.

In Figure 5.1 we have plotted  $\log_{10}(\|\hat{T}_n\|)$  and  $\log_{10}(\|T_n\|)$  at different points for explicit methods of 1 to 5 steps. In Figure 5.2 the same is done for the implicit methods. The curves in these figures indicate the same general behaviour of the local truncation error norms as in the earlier chapters.

In Table 5.9 we present the end point ( $x_N=1.2$ ) errors in the numerical solution of the twenty four differential equations by five step usual, optimal ( $\hat{M}$ ), optimal interpolatory for polynomials ( $\hat{M}^1, \hat{M}^2, \dots$ , etc., the superscript denoting the degree of the polynomials) and optimal interpolatory for  $\exp(1.6x)$ ,  $\exp(-1.6x)$  (denoted as  $\hat{M}^F$ )-methods, in the explicit case. We observe that for these explicit methods the error is least for the method:  $\hat{M}$  on equations 11, 12, 17, 18, 19, 21 and 22;  $\hat{M}^1$  on equation 9;  $\hat{M}^2$  on 1, 3, 4 and 6;  $\hat{M}^3$  on equations 20 and 23;  $\hat{M}^4$  on equation 24; and  $\hat{M}^F$  on equations 2, 5, 7, 8, 10, 13, 14, 15 and 16.

In Table 5.10 we, similarly, present the end point ( $x_N=1.2$ ) errors for the implicit methods  $\hat{M}, \hat{M}^1, \dots, \hat{M}^5$  and  $\hat{M}^F$ . We observe that the error is least for:  $\hat{M}$  on equations 3, 6, 7, 8, and 9;  $\hat{M}^1$  on 11, 12, 19, 21 and 22;  $\hat{M}^2$  on equations 18, 20, 24;  $\hat{M}^3$  on equation 17;  $\hat{M}^4$  on equations 13 and 23;

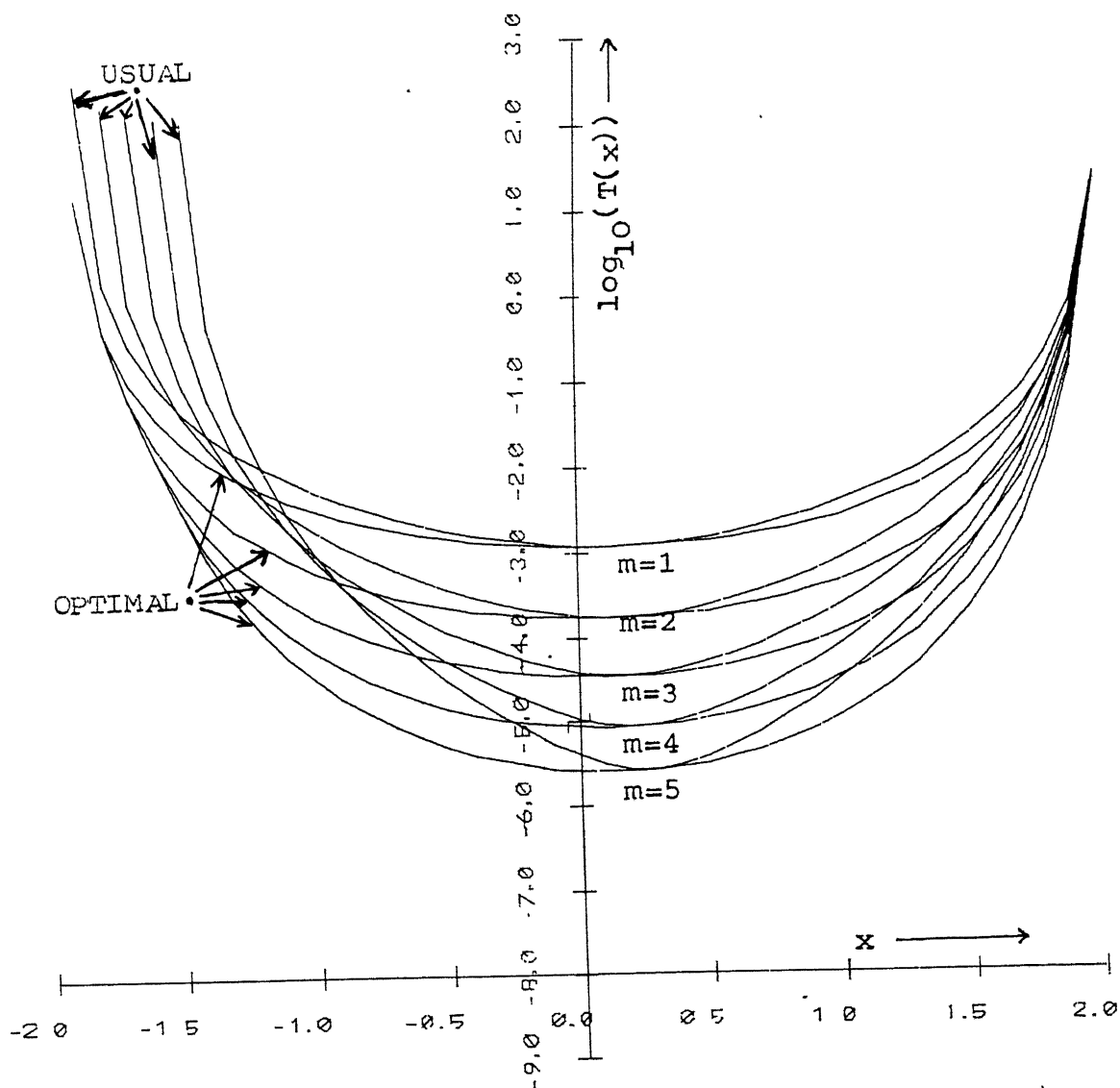


Figure 5.1: Local Truncation Error in Explicit  $L^2(\hat{c}_r)$  -  
Optimal Multistep Methods/Usual Methods  
( $r=2.01$ ,  $h=0.1$ )

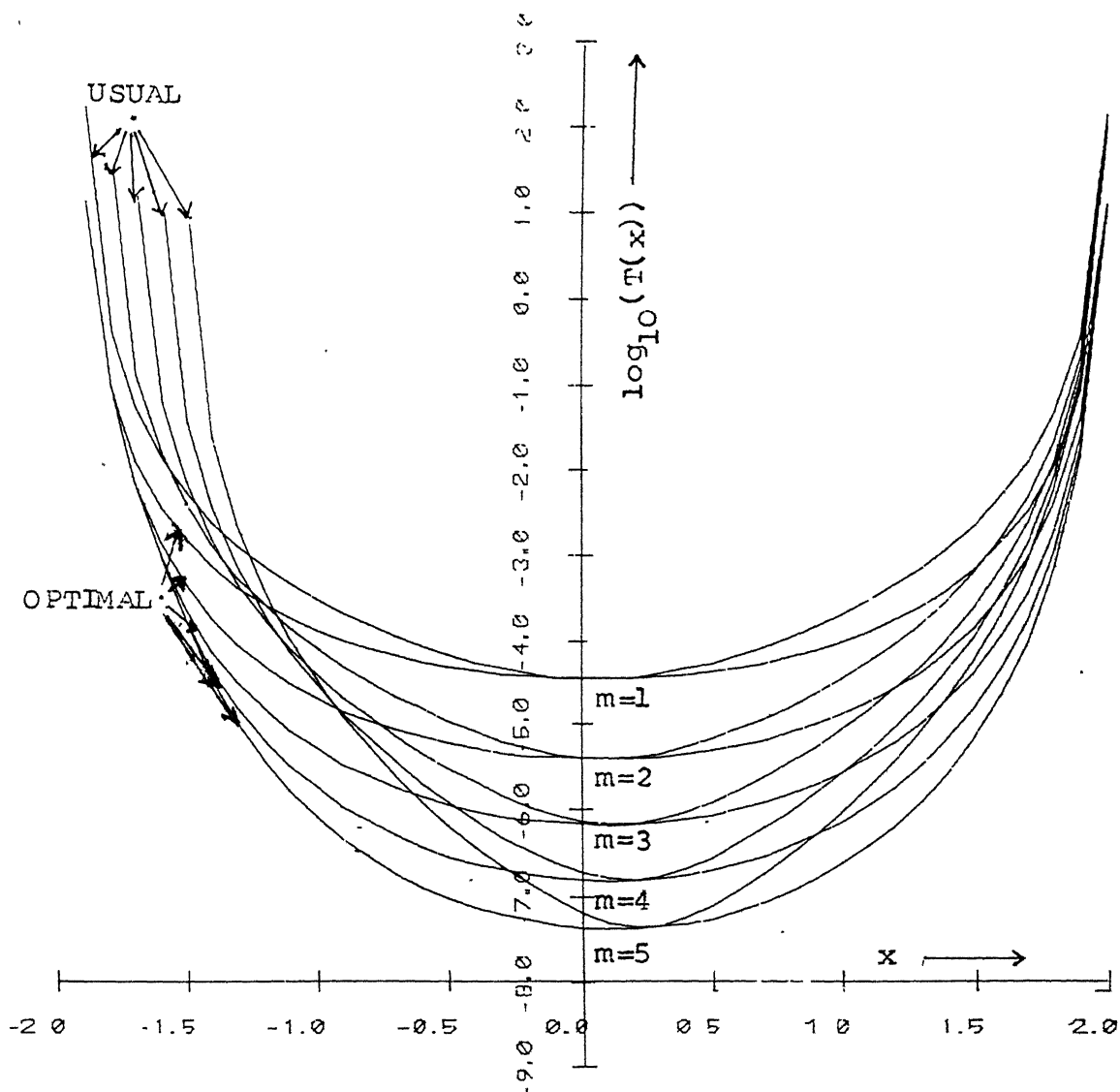


Figure 5.2: Local Truncation Error in Implicit  $L^2(\hat{C}_r)$ -  
Optimal Multistep Methods/Usual Methods  
( $r=2.01$ ,  $h=0.1$ )

End point ( $x_N=1.2$  errors for explicit  $L^2(\hat{c}_r)$ -optimal  
Multistep methods

Eqn. no.	Usual	$\hat{M}$	$\hat{M}^1$	Methods $\hat{M}^2$	$\hat{M}^3$	$\hat{M}^4$	$\hat{M}^F$
1	-.27E-02	-.66E-04	-.11E-03	.12E-04	-.19E-03	.19E-03	-.31E-04
2	-.93E-02	-.44E-04	-.78E-04	.25E-04	-.11E-03	.17E-03	-.12E-04
3	-.61E-03	-.10E-03	-.14E-03	-.23E-04	-.33E-03	.22E-03	-.65E-04
4	-.24E-02	-.60E-04	-.92E-04	.16E-04	-.19E-03	.29E-03	-.20E-04
5	.30E-02	.17E-03	.34E-03	-.87E-04	.34E-03	-.42E-03	.82E-04
6	-.97E-03	-.11E-04	-.11E-04	-.70E-06	-.48E-04	.14E-04	-.37E-05
7	-.16E-03	-.98E-06	-.79E-06	-.38E-06	-.79E-05	.29E-05	-.24E-06
8	.92E-03	-.14E-04	-.13E-04	-.13E-04	-.64E-04	.61E-04	.60E-05
9	-.37E-03	-.17E-05	-.54E-06	.24E-05	-.25E-04	.26E-04	.30E-05
10	-.48E-01	-.25E-02	-.30E-02	.32E-03	-.12E-01	.21E-01	-.29E-03
11	-.33E+02	.11E+00	-.10E+01	.27E+02	-.51E+02	.48E+02	.21E+02
12	.33E+02	-.11E+00	.24E+00	-.28E+02	.50E+02	-.49E+02	-.21E+02
13	-.16E-04	-.13E-04	.30E-04	.89E-05	-.15E-04	.12E-04	-.75E-05
14	.10E-04	-.12E-04	.26E-04	.75E-05	-.12E-04	.84E-05	-.72E-05
15	-.22E-04	-.10E-04	.22E-04	.83E-05	-.17E-04	.15E-04	-.35E-05
16	-.15E-04	-.90E-05	-.19E-04	.70E-05	-.13E-04	.11E-04	-.35E-05
17	-.70E-07	.46E-08	.11E-07	.27E-07	-.68E-07	.66E-07	.29E-07
18	-.52E-06	.47E-07	.11E-06	.28E-06	-.67E-06	.59E-06	.30E-06
19	.70E-02	.15E-03	.60E-03	.82E-03	-.38E-03	-.64E-03	.59E-03
20	-.14E-02	.12E-04	.80E-04	.19E-03	.67E-05	.19E-04	.15E-03
21	-.13E-C2	.86E-06	.92E-04	.15E-03	-.22E-04	.48E-04	.16E-03
22	.24E-02	.35E-04	.27E-03	.37E-03	-.20E-03	.85E-04	.32E-03
23	.27E-C2	.35E-C3	.11E-02	.45E-03	-.24E-03	-.76E-03	.80E-03
24	-.71E-C4	.10E-04	.62E-04	.84E-04	.35E-04	-.89E-05	.90E-04

Table 5.10

End point ( $x_N=1.2$ ) errors for implicit  $L^2(\hat{C}_r)$ -optimal multistep methods

( $r=2.01$ ,  $h=0.1$ )

Eqn. No.	Usual	Methods						
		$\hat{M}$	$\hat{M}_1$	$\hat{M}_2$	$\hat{M}_3$	$\hat{M}_4$	$\hat{M}_5$	$\hat{M}_F$
1	-.82E-04	.51E-06	.10E-05	-.10E-05	.12E-05	-.44E-05	.57E-05	.15E-07
2	-.26E-04	.56E-06	-.10E-05	-.69E-06	.12E-05	-.22E-05	.48E-05	.25E-06
3	-.19E-03	.23E-06	.67E-06	-.16E-05	.11E-05	-.84E-05	.79E-05	-.56E-06
4	-.69E-04	.50E-06	.91E-06	-.88E-06	.16E-05	-.41E-05	.92E-05	.26E-07
5	.86E-04	-.26E-05	-.49E-05	.25E-05	-.33E-05	.66E-05	-.11E-04	-.18E-05
6	-.32E-04	-.92E-07	-.13E-06	-.37E-06	.28E-07	-.13E-05	.57E-06	-.34E-06
7	-.53E-05	-.28E-07	-.33E-07	-.36E-07	.34E-07	-.21E-06	.91E-07	-.38E-07
8	-.29E-04	-.89E-07	-.17E-06	-.60E-06	.32E-06	-.15E-05	.19E-05	-.54E-06
9	-.12E-04	-.82E-07	-.97E-07	-.91E-07	.25E-06	-.56E-06	.75E-06	-.10E-06
10	-.67E-03	.11E-04	.18E-04	-.23E-04	.12E-03	-.27E-03	.48E-03	-.70E-05
11	-.39E+00	.29E-01	-.92E-02	-.36E+00	.95E 00	-.10E+01	.72E+00	-.24E+00
12	.39E+00	.68E-01	.41E-01	.38E+00	.94E 00	.10E+01	-.72E+00	.26E+00
13	-.18E-06	.26E-06	.50E-06	-.18E-06	.22E-06	-.17E-06	.18E-06	.23E-06
14	-.12E-06	.23E-06	.44E-06	-.16E-06	.16E-06	-.13E-06	.11E-06	.22E-06
15	-.28E-06	.18E-06	.33E-06	-.18E-06	.22E-06	-.22E-06	.25E-06	.12E-06
16	-.18E-06	.16E-06	.30E-06	-.15E-06	.18E-06	-.16E-06	.18E-06	.11E-06
17	-.84E-09	.35E-09	-.38E-06	-.25E-09	.14E-08	-.93E-09	.70E-09	-.28E-09
18	-.51E-08	.19E-08	-.19E-08	-.93E-09	.14E-07	-.75E-08	.70E-08	-.14E-08
19	-.22E-03	.14E-04	.30E-05	-.82E-05	-.84E-05	-.17E-04	.38E-05	-.19E-04
20	-.46E-04	.44E-05	-.24E-05	-.69E-07	-.63E-06	.32E-05	.39E-06	-.22E-05
21	-.32E-04	.28E-05	.56E-06	-.15E-05	-.98E-06	-.30E-05	-.18E-05	-.39E-05
22	-.72E-04	.35E-05	-.18E-05	-.63E-05	-.35E-05	-.71E-05	.49E-05	-.12E-04
23	.77E-04	-.41E-05	-.18E-04	-.94E-05	-.11E-04	-.24E-05	-.12E-04	-.28E-04
24	.21E-05	.27E-05	.14E-05	-.25E-06	-.38E-06	-.82E-06	-.35E-06	-.12E-05

## CHAPTER 6

### ERROR ANALYSIS OF OPTIMAL MULTISTEP METHODS

#### 6.1 Introduction

This chapter is a study of certain theoretical aspects of the optimal multistep methods discussed in the previous chapters. These aspects concern convergence, magnitude of discretization error and propagation of round offs in the implementation of the optimal and quadrature optimal multistep methods. The study also includes the optimal and quadrature optimal methods which are interpolatory for polynomials of a certain degree.

The results obtained in this chapter establish the applicability of our methods to a general situation in which the solution does not necessarily belong to the underlying Hilbert space.

In Section 6.2 we prove that the coefficients of optimal multistep methods as well as those of quadrature optimal multistep methods approach the coefficients of the related usual methods as  $h \rightarrow 0$ . This holds also if the optimal/quadrature optimal methods are interpolatory for polynomials of certain degree. In Section 6.3 we state some results from Henrici [27] which are required in the subsequent sections. In Section 6.4 we give an estimate

for local truncation error. In Section 6.5 convergence of these methods is established, while in Section 6.6 a bound on discretization error and in section 6.7 a bound on round off error propagation have been derived.

Throughout this chapter,  $H$  denotes either of the spaces  $H^2(c_r)$  or  $L^2(\hat{c}_r)$  as described in chapters 2 and 4. The points  $x_i$ 's satisfying  $a=x_0 < x_1 < \dots < x_N=b$  are assumed to be equispaced with spacing  $h$ . The interval  $[a,b]$  of integration is a subset of the open interval  $(-r,r)$ . An  $m$ -step method would then start from the point  $x_m$  and will calculate the solution at the points  $x_m$  through  $x_N$ . Note that  $N$  is a function of  $h$  so that  $Nh = b-a$ .

In the sequel an  $H$ -optimal multistep method commonly denotes any of optimal/quadrature optimal/interpolatory for polynomials of specified degree methods, implicit or explicit.

Our main concern in the earlier chapters has been the computation of coefficients of multistep formulae for a fixed set of nodes. In this chapter, however, we need to stress the dependence of the coefficients  $b_j$ 's on the current variable point  $x_{n+1}$  in the integration scheme. For this reason the dependence of  $b_j$ 's on the point  $x_{n+1}$  is indicated by writting them as  $b_{j,n+1}$ 's. In section 6.3 onwards, where a slight change of notations

occurs, the dependence of coefficients  $\beta_j$ 's on the point has been denoted by presence of a subscript  $m$  in  $\beta_{jm}$  where  $x_m$  is the farthest point from the current point  $x_{m+k}$  in a  $k$  step formula.

## 6.2 Magnitude of the Coefficients in H-optimal Multistep Methods

The following two lemmas relate the coefficients in a H-optimal multistep formula with the coefficients of the corresponding usual formula.

Lemma 1. Let

$$(1) \quad y_{n+1} = y_{n-s} + h \sum_{j=\delta_{t0}}^m \tilde{b}_{j,n+1} f(x_{n+1-j}, y_{n+1-j}), \quad s < m, \quad m-1 \leq n \leq N-1,$$

be an  $m$ -step quadrature optimal multistep method/interpolatory for polynomials of degree  $p < m + \delta_{t1}$  in  $H$  and let

$$(2) \quad y_{n+1} = y_{n-s} + h \sum_{j=\delta_{t0}}^m b_j f(x_{n+1-j}, y_{n+1-j}), \quad s < m, \quad m-1 \leq n \leq N-1,$$

denote the corresponding usual multistep method. Then, uniformly for  $m-1 \leq n \leq N-1$ ,

$$|\tilde{b}_{j,n+1} - b_j| = O(h), \quad h \rightarrow 0, \quad j = \delta_{t0}(1)m.$$

Proof: The methods (1) and (2) are implicit if  $t=1$  and explicit if  $t=0$ . Correspondingly let us consider polynomials



$$(3) \quad L_{in}(x) = \prod_{\substack{j=\delta_{to} \\ j \neq i}}^m \frac{x_{n+1-i} - x_{n+1-j}}{x_{n+1-i} - x_{n+1-j}}, \quad m-1 \leq n \leq N-1, \quad \delta_{to} \leq 1 \leq m$$

As  $x_{n+1-j}$ 's belong to  $[a, b]$  and they are equispaced, the norm of the polynomial  $L_{in}$  in  $H$  satisfies

$$(4) \quad \|L_{in}\| = O(h^{-(m-\delta_{to})}),$$

uniformly in  $i$  and  $n$ . Since the formula (2) is exact for polynomials of degree  $m+1-\delta_{to}$  we have

$$hb_j = \int_{x_{n-s}}^{x_{n+1}} L_{jn}(x) dx, \quad j=\delta_{to}(1)m.$$

Applying the method (1) on  $L_{jn}(x)$  and using Lemma 5 of the next section (Lemma 5.7, Henrici [27])

$$\begin{aligned} \left| \int_{x_{n-s}}^{x_{n+1}} L_{jn}(x) dx - h \tilde{b}_{jn+1} \right| &\leq \|L_{jn}\| \|\tilde{Q}_n\| \\ &\leq \|L_{jn}\| \|Q_n^u\| \\ &\leq C_t \|L_{jn}\| h^{m+2-\delta_{to}} M_{m+1-\delta_{to}, s} \\ &= O(h^2) \end{aligned}$$

uniformly in  $n$  where, in view of Theorems 2.1 and 4.1,

$$M_{m+1-\delta_{to}} = \max_{x \in [a, b]} \|D_x^{m+1-\delta_{to}}\| < \infty,$$

$D_x^{m+1-\delta_{to}}$  denotes the derivative evaluation functional of order  $m+1-\delta_{to}$  and  $\tilde{Q}_n$  and  $Q_n^u$  designate the quadrature

error functionals in the optimal and usual cases, respectively, corresponding to the point  $x_{n+1}$ . Hence

$$(5) \quad |\tilde{b}_{j,n+1} - b_j| = O(h), \quad h \rightarrow 0,$$

uniformly in  $j = \delta_{t0}(1)m$ ,  $m-1 \leq n \leq N-1$ , completing the proof.

Lemma 2: Let

$$(6) \quad y_{n+1} = \sum_{i=1}^m a_i y_{n+1-i} + h \sum_{j=\delta_{t0}}^m \hat{b}_{j,n+1} f(x_{n+1-j}, y_{n+1-j}),$$

$$m-1 \leq n \leq N-1$$

be an optimal multistep method/interpolatory for polynomials of degree  $p < m + \delta_{t1}$  in  $H$  and let

$$(7) \quad y_{n+1} = \sum_{i=1}^m a_i y_{n+1-i} + h \sum_{j=t0}^m b_j f(x_{n+1-j}, y_{n+1-j}),$$

$$m-1 \leq r \leq N-1,$$

be the corresponding usual method. Then, uniformly for  $m-1 \leq n \leq N-1$ ,

$$|\hat{b}_{j,n+1} - b_j| = O(h), \quad h \rightarrow 0, \quad j = \delta_{t0}(1)m.$$

Proof: As before  $t = 1$  refers to an implicit and  $t = 0$  to an explicit case. Let

$$(8) \quad M_{in}(x) = \int_a^x L_{in}(s) ds, \quad \delta_{t0} \leq i \leq m, \quad m-1 \leq n \leq N-1,$$

where  $L_{in}(s)$  is as defined in (3). It follows from (4) that

$$(9) \quad \|M_{in}\| = O(h^{-(m-\delta_{to})})$$

uniformly in  $i$  and  $n$ . Since the usual formula (7) is exact for polynomials of degree  $m+\delta_{t1}$ , applying it on  $M_{in}(x)$  we get

$$h b_j = M_{jn}(x_{n+1}) - \sum_{i=1}^m a_i M_{jn}(x_{n+1-i}).$$

Next, by applying the optimal formula (5) on  $M_{jn}(x)$  and reasoning as in the proof of Lemma 1, we get

$$\begin{aligned} |M_{jn}(x_{n+1}) - \sum_{i=1}^m a_i M_{jn}(x_{n+1-i}) - h \hat{b}_{j,n+1}| \\ \leq \|M_{jn}\| \|\hat{T}_n\| \\ \leq \|M_{jn}\| \|T_n\| \\ \leq \|M_{jn}\| C_t^0 h^{m+2-\delta_{to}} M_{m+1-\delta_{to}}, \text{ say} \\ = O(h^2) \end{aligned}$$

uniformly in  $m-1 \leq n \leq N-1$ . Here

$$M_{m+1-\delta_{to}} = \max_{x \in [a,b]} \|D_x^{m+1-\delta_{to}}\|,$$

$[a,b]$  is the interval of integration and  $\hat{T}_n$  and  $T_n$  denote the local truncation error functionals corresponding to the point  $x_{n+1}$  in the optimal and usual cases, respectively. Thus, we have

$$(10) \quad |b_{j,n+1} - b_j| = O(h),$$

uniformly in  $m-1 \leq n \leq N-1$ .

### 6.3 Some Auxiliary Results

In this section we state three results from Henrici [27] which are to be used in our later analysis.

Let

$$(11) \quad L(y(x);h) = \alpha_k y(x+kh) + \alpha_{k-1} y(x+(k-1)h) + \dots + \alpha_0 y(x) \\ - h \{ \beta_k y'(x+kh) + \beta_{k-1} y'(x+(k-1)h) + \dots + \beta_0 y'(x) \}$$

be a difference operator. The operator  $L(y(x);h)$  corresponds to a general  $k$ -step method given by

$$(12) \quad \alpha_k y_{m+k} + \alpha_{k-1} y_{m+k-1} + \dots + \alpha_0 y_m \\ = h \{ \beta_k f_{m+k} + \dots + \beta_0 f_m \}$$

where

$$f_{m+i} = f(x_{m+i}, y_{m+i}) \quad , \quad i = 0(1)k .$$

Here, if  $\beta_k = 0$  the method is explicit and it is implicit otherwise.

The difference operator  $L$ , or the method (12), is said to be of order  $p$  if

$$(13) \quad \sum_{i=0}^k \alpha_i = 0 ,$$

$$(14) \quad \sum_{i=1}^k i^q \alpha_i = q \sum_{j=1}^k j^{q-1} \beta_j \quad , \quad q = 1(1)p ,$$

and

$$(15) \quad \sum_{i=1}^k i^{p+1} \alpha_i \neq (p+1) \sum_{j=1}^k j^p \beta_j .$$

A multistep method given by (12) is called consistent if

$$(16) \quad \rho(1) = 0,$$

and

$$(17) \quad \rho'(1) = \sigma(1),$$

where

$$(18) \quad \rho(\zeta) = \alpha_k \zeta^k + \alpha_{k-1} \zeta^{k-1} + \dots + \alpha_0,$$

and

$$(19) \quad \sigma(\zeta) = \beta_k \zeta^k + \beta_{k-1} \zeta^{k-1} + \dots + \beta_0$$

are the associated polynomials of multistep formula (12). The conditions (16)-(17) amount to saying that the formula (12) is locally exact for polynomials of degree one, or that the order  $p$  of (12) is at least one.

The formula (12), or the method associated with it, where  $\alpha_0, \alpha_1, \dots, \alpha_k$  are prefixed, is 'usual' if the  $\beta_j$ 's are chosen so as to maximize the order of the method. Note that for a usual  $k$ -step method the order is at least  $k$  in the explicit case and  $k+1$  in the implicit case.

Lemma 3: Let the polynomial  $\rho(\zeta) = \alpha_k \zeta^k + \alpha_{k-1} \zeta^{k-1} + \dots + \alpha_0$  satisfy the condition of stability and let the coefficients  $\gamma_l$  ( $l=0, 1, 2, \dots$ ) be defined by

$$\frac{1}{\alpha_k + \alpha_{k-1} \zeta + \dots + \alpha_0 \zeta^k} = \gamma_0 + \gamma_1 \zeta + \gamma_2 \zeta^2 + \dots$$

Then,

$$(20) \quad \Gamma = \sup_{l=0,1,\dots} |\gamma_l| < \infty.$$

Lemma 4. Let the polynomial  $\rho(\zeta) = \alpha_k \zeta^k + \dots + \alpha_0$  satisfy the condition of stability, let  $B^*$ ,  $\beta$  and  $\Lambda$  be nonnegative constants such that

$$(21) \quad |\beta_{k,n}| + |\beta_{k-1,n}| + \dots + |\beta_{0,n}| \leq B^*,$$

$$|\beta_{k,n}| \leq \beta, \quad |\lambda_n| \leq \Lambda, \quad n=0,1,2,\dots,N$$

and let  $0 \leq h < \alpha_k \beta^{-1}$ . Then, every solution of

$$(22) \quad \alpha_k z_{m+k} + \alpha_{k-1} z_{m+k-1} + \dots + \alpha_0 z_m$$

$$= h \{ \beta_{k,m} z_{m+k} + \beta_{k-1,m} z_{m+k-1} + \dots + \beta_{0,m} z_m \} + \lambda_m z_m$$

for which

$$(23) \quad |z_\mu| \leq Z, \quad \mu = 0,1,\dots,k-1,$$

satisfies

$$(24) \quad |z_n| \leq K^* e^{nhL^*}, \quad n = 0,1,\dots,N,$$

where

$$(25) \quad L^* = \Gamma^* B^*, \quad K^* = \Gamma^* (N\Lambda + AZ_k),$$

$$(26) \quad A = |\alpha_k| + |\alpha_{k-1}| + \dots + |\alpha_0|$$

and

$$\Gamma^* = \frac{\Gamma}{1+h|\alpha_k|^{-1}\beta}.$$

Lemma 5. Let  $L(y(x);h)$  be a difference operator of order  $p>0$ . There exists a constant  $G>0$  depending

only on  $L$ , such that

$$(27) \quad |L(y(x); h)| \leq h^{p+1} GY \quad a \leq x, x+kh \leq b$$

for all functions  $y(x)$  having a continuous derivative of order  $p+1$  in  $[a, b]$  with  $Y = \max_{x \in [a, b]} |y^{(p+1)}(x)|$ .

#### 6.4 A Bound for Local Truncation Error

A generalization of Lemma 5, applicable to  $H$ -optimal methods, is as follows:

Lemma 6. Let  $L(y(x); h)$  given by (11) be the difference operator of a  $k$ -step usual method of order  $p$  and let

$$(28) \quad L_x^0(y(x); h) = \alpha_k y(x+kh) + \alpha_{k-1} y(x+(k-1)h) + \dots + \alpha_0 y(x) \\ - h \{ \beta_{k,x}^0 y'(x+kh) + \dots + \beta_{0,x}^0 y'(x) \}$$

denote the difference operator of a corresponding  $H$ -optimal  $k$ -step method (the subscript  $x$  in  $\beta_{j,x}^0$  denoting the dependence of these coefficients on  $x$ ). Let  $y$  possess a continuous derivative of order  $p+1$  on the interval  $[a, b]$  and set

$$(29) \quad Y = \max_{\substack{x \in [a, b] \\ 0 \leq i \leq p+1}} |y^{(i)}(x)|$$

Then

$$\begin{aligned}
 (30) \quad & |\alpha_k y(x+kh) + \alpha_{k-1} y(x+(k-1)h) + \dots + \alpha_0 y(x) \\
 & - h\{\beta_{0,x}^0 y'(x+kh) + \dots + \beta_{0,x}^0 y'(x)\}| \\
 & = |L_x^0(y(x); h)| \leq h^{p+1} G^* y,
 \end{aligned}$$

uniformly in  $x$ ,  $x+kh \in [a, b]$  where  $G^*$  is a constant independent of  $y$ .

Proof: We know that

$$\begin{aligned}
 (31) \quad y(t) &= y(x) + (t-x)y'(x) + \dots + \frac{1}{p!}(t-x)^p y^{(p)}(x) + \frac{1}{p!} \int_x^t (t-s)^p y^{(p+1)}(s) ds \\
 &= P(t) + Q(t), \text{ say.}
 \end{aligned}$$

Then, if (26) is an optimal method/interpolatory for polynomials of a certain degree (as distinguished from a quadrature optimal case) and  $||L_x^0||$ ,  $||L_x||$  respectively denote the norms of the functionals  $L_x^0$  and  $L$  corresponding to the current point  $x+kh$ , we have

$$\begin{aligned}
 (32) \quad |L_x(P(x); h)| &\leq ||P|| \quad ||L_x^0|| \\
 &\leq ||P|| \quad ||L_x|| \\
 &\leq (C_1 y) (C_2 M_{p+1} h^{p+1}),
 \end{aligned}$$

using Lemma 5 and (29) (for estimating  $||P||$ ), where

$$M_{p+1} = \max_{x \in [a, b]} ||D_x^{p+1}||,$$

and  $C_1, C_2$  are constants not depending on  $x$ .



By directly substituting the expression for  $Q(x)$  in (28) and simplifying we get

$$(33) \quad |L_x^0(Q(x);h)| \leq C_3 Y M_{p+1} h^{p+1},$$

where  $C_3$  is a constant independent of  $x$ . From (31), (32) and (33) it follows that

$$(34) \quad |L_x^0(y(x);h)| \leq h^{p+1} G^* Y,$$

where we have set

$$G^* = (C_1 C_2 + C_3) M_{p+1}.$$

This proves the result in the optimal case.

If the method corresponding to the operator  $L_x^0$  in (28) represents a quadrature optimal method/interpolatory for polynomials of a certain degree, rewriting  $L_x^0$  and  $L_x$  temporarily as  $\tilde{L}_x^q$  and  $L_x^q$ , respectively, and regarding these as quadrature error functionals corresponding to the current point  $x+kh$ , we have

$$\begin{aligned} (35) \quad |L_x^0(P(x);h)| &\leq \|P'\| \|\tilde{L}_x^q\| \\ &\leq \|P'\| \|L_x^q\| \\ &\leq (C_4 Y) (C_5 h^{p+1} M_p) \end{aligned}$$

where  $C_4$  and  $C_5$  are constants independent of  $x$ , and

$$M_p = \max_{x \in [a,b]} \|D_x^p\|.$$

Also, by a direct substitution, we have

$$(36) \quad |L_x^0(Q(x);h)| \leq C_6 Y h^{p+1} M_p,$$

the constant  $C_6$  being independent of  $x$ . Combining (31), (35) and (36), we get

$$(37) \quad |L_x^0(y(x);h)| \leq h^{p+1} G^* Y,$$

where we have put  $G^* = (C_4 C_5 + C_6) M_p$ .

Hence, from (34) and (37), the result is valid for any H-optimal method.

### 6.5 Convergence of H-optimal Methods

Let  $f(x,y)$  satisfy the following conditions:

- (A)  $f(x,y)$  is defined and continuous in the strip  $a \leq x \leq b$ ,  $-\infty < y < \infty$ , where  $a, b$  are finite.
- (B) For any two numbers  $y$  and  $y^*$  and  $x \in [a, b]$ , a constant  $L$  exists such that

$$|f(x,y) - f(x,y^*)| \leq L |y - y^*|.$$

Then, a linear multistep method

$$(38) \quad \alpha_k y_{n+k} + \alpha_{k-1} y_{n+k-1} + \dots + \alpha_0 y_n \\ = h \{ \beta_{kn} f_{n+k} + \beta_{k-1n} f_{n+k-1} + \dots + \beta_{0n} f_n \}$$

where  $f_m = f(x_m, y_m)$  ( $m=0, 1, 2, \dots$ ), with  $|\alpha_k| \neq 0$  and  $|\alpha_0| + |\beta_{0n}| > 0$ , is called convergent if for all

functions  $f(x,y)$  satisfying the conditions (A) and (B) and for all values of  $\eta$  there holds

$$(39) \quad \lim_{\substack{h \rightarrow 0 \\ x_n = x}} y_n = y(x)$$

for all  $x \in [a,b]$  and all solutions  $\{y_n\}$  of the difference equation (38) having starting values  $y_\mu = \eta_\mu(h)$  satisfying

$$(40) \quad \lim_{h \rightarrow 0} \eta_\mu(h) = \eta, \quad \mu = 0, 1, \dots, k-1,$$

where  $y(x)$  denotes the solution of the initial value problem

$$(41) \quad \frac{dy}{dx} = f(x,y), \quad y(a) = \eta.$$

The criterion of convergence described above is similar to that given by Henrici [27, p. 217].

We now prove:

Theorem 1: An H-optimal method corresponding to a stable and consistent usual multistep method is convergent.

Proof. Let

$$(42) \quad \delta = \delta(h) = \max_{\mu=0,1,\dots,k-1} \|\eta_\mu(h) - y(a+\mu h)\|$$

with

$$\lim_{h \rightarrow 0} \delta(h) = 0.$$

Let the difference operators in the usual and H-optimal

cases be denoted by  $L(y(x);h)$  and  $L_x^H(y(x);h)$ , respectively. In view of Lemmas 1-2 we have  $|\beta_{jm}^H - \beta_j| = O(h)$  where  $\beta_{jm}^H$ 's are the coefficients of the H-optimal method occurring in  $L_x^H(y(x);h)$  corresponding to  $x = x_{m+k}$ . With  $\|y'\| = \max_{x \in [a,b]} |y'(x)|$ , we have

$$\begin{aligned}
 (43) \quad |L_x^H(y(x);h) - L(y(x);h)| \\
 \leq h \sum_{j=0}^k |\beta_{jm}^H - \beta_j| \|y'\| \\
 = O(h^2),
 \end{aligned}$$

uniformly in  $x \in [a, b-kh]$ . Since  $L$  is consistent and  $y' = f(x, y(x))$  is continuous in  $[a, b]$ ,

$$(44) \quad |L(y(x);h)| = O(h),$$

uniformly in  $x \in [a, b-kh]$ . Therefore

$$(45) \quad |L_x^H(y(x);h)| \leq h\theta(h)$$

where  $\theta(h) \rightarrow 0$  as  $h \rightarrow 0$  and is independent of  $x \in [a, b-kh]$ . Thus with

$$(46) \quad e_m = y_m - y(x_m), \quad m=0, 1, 2, \dots$$

and

$$(47) \quad g_m = \begin{cases} [f(x_m, y_m) - f(x_m, y(x_m))] e_m^{-1}, & \text{if } e_m \neq 0 \\ 0, & \text{if } e_m = 0, \end{cases}$$

we have

$$\begin{aligned}
 (48) \quad & \alpha_k e_{m+k} + \dots + \alpha_0 e_m \\
 & - h \{ \beta_{km}^H g_{m+k} e_{m+k} + \dots + \beta_{0m}^H g_m e_m \} \\
 & = \theta_m h \quad \theta(h)
 \end{aligned}$$

where  $|\theta_m| \leq 1$ . The definition (47) of  $g_m$ , in view of the Lipschitz condition (B) as stated in the definition of convergence, implies that

$$|g_m| \leq L, \quad m = 0, 1, 2, \dots$$

Applying Lemma 4, with  $z_m = e_m$ ,  $Z = \delta(h)$ ,  $\Lambda = h\theta(h)$ ,  $N = (x_n - a)/h$  and  $B^* = BL$  where

$$(49) \quad B = \sup_{m,h} \{ |\beta_{0m}^H| + |\beta_{1m}^H| + \dots + |\beta_{km}^H| \} < \infty,$$

(by Lemmas 1-2), we have

$$e_n \leq \Gamma^* [(x_n - a)\theta(h) + A\delta(h)k] \exp[(x_n - a)\Gamma^* B^*]$$

where

$$\Gamma^* = \frac{\Gamma}{1 + h|\alpha_k|^{-1} \beta L},$$

with  $\beta = \sup \{ |\beta_{km}^H| : m, h \} < \infty$  (by Lemmas 1-2),  $A$  as in (26) and  $\Gamma$  as in (20). Since  $\theta(h) \rightarrow 0$  and  $\delta(h) \rightarrow 0$  as  $h \rightarrow 0$  we have  $|e_n| \rightarrow 0$  as  $h \rightarrow 0$ . This completes the proof.

## 6.6 A Bound for the Discretization Error

Let us assume that the exact solution  $y(x)$  has a continuous derivative of order  $p+1$  on  $[a,b]$ , with

$$(50) \quad Y = \max_{x \in [a,b]} \sum_{i=0}^{p+1} |y^{(i)}(x)|.$$

With the milder assumption

$$(51) \quad \alpha_k y_{m+k} + \alpha_{k-1} y_{m+k-1} + \dots + \alpha_0 y_n \\ - h \{ \beta_{km} f_{m+k} + \dots + \beta_{om} f_m \} = \theta_m K_1 h^{q+1}$$

where  $K_1$  and  $q$  are non-negative constants and  $|\theta_m| \leq 1$  (rather than the exact satisfaction of the difference scheme), we have the following a priori bound on the discretization error:

Theorem 2: If  $h$  is such that  $h |\beta_k^* \alpha_k^{-1}| L < 1$ , where  $\beta_k^* = \max \{ \beta_{km} : m \}$  and  $x_n \in [a,b]$ ,

$$|e_n| \leq \Gamma^* [A \delta k + (x_n - a) (K_1 h^{q+G^*} Y h^p)] \exp (x_n - a) L \Gamma^* B]$$

where

$$(52) \quad \Gamma^* = \frac{\Gamma}{1 - h |\alpha_k^{-1} \beta_k^*| L}$$

and  $\delta$ ,  $A, G^*$ ,  $\Gamma$  and  $B$  are as in (42), (26), (30), (20) and (49), respectively.

Proof. Subtracting  $L_{x_m}^H (y(x_m); h)$  from (51) we have

$$\alpha_k e_{m+k} + \dots + \alpha_0 e_m - h \{ \beta_{km}^H g_{m+k} e_{m+k} + \dots + \beta_{0m}^H g_m e_m \} \\ = \bar{\theta}_m [K_1 h^{q+1} + G^* Y h^{p+1}] , \quad m=0,1,2,\dots$$

by Lemma 6, where  $|\bar{\theta}_m| \leq 1$ . The theorem now follows by an application of Lemma 4.

Note that if  $\delta(h) = O(h^p)$  and  $q \geq p$  then  $e_n = O(h^p)$ .

### 6.7 An a Priori Bound on Round off Errors

To study the influence of local round off errors, instead of the exact difference scheme

$$\alpha_k y_{n+k} + \dots + \alpha_0 y_n = h \{ \beta_{kn}^H f(x_{n+k}, y_{n+k}) + \dots + \beta_{0n}^H f(x_n, y_n) \},$$

let the quantities  $\tilde{y}_n$ , actually calculated, satisfy

$$\alpha_k \tilde{y}_{n+k} + \dots + \alpha_0 \tilde{y}_n = h \{ \beta_{kn}^H f(x_{n+1}, \tilde{y}_{n+k}) + \dots + \beta_{0n}^H f(x_n, \tilde{y}_n) \} + \\ + \varepsilon_{n+k}, \quad n=0,1,2,\dots$$

where the quantities  $\varepsilon_n$  are the local round off errors with

$$|\varepsilon_{n+k}| \leq \varepsilon, \quad n = 0,1,2,\dots,$$

where  $\varepsilon$  is a constant.

An a priori bound for the accumulated round off errors  $r_n = \tilde{y}_n - y_n$  is, then, given by the following:

Theorem 3: With  $h$  and  $\beta_k^*$  as in Theorem 2,

$$|r_n| \leq \varepsilon h^{-1} (x_n - a) \Gamma^* \exp[(x_n - a) \Gamma^*_{BL}], \quad n=k, k+1, \dots$$

where  $l^*$  is as in (52),  $B$  is as in (49) and  $L$  is the Lipschitz constant for the function  $f(x,y)$  in (B).

Proof. Along the lines of the proof of Theorem 2, if

$$g_m = \begin{cases} r_m^{-1} [f(x_m, \tilde{y}_m) - f(x_m, y_m)], & \text{if } r_m \neq 0 \\ 0, & \text{if } r_m = 0, \end{cases}$$

we have

$$\begin{aligned} & \alpha_k r_{n+k} + \alpha_{k-1} r_{n+k-1} + \dots + \alpha_0 r_n \\ &= h \{ \beta_{kn}^H g_{n+k} r_{n+k} + \dots + \beta_{0n}^H g_n r_n \} + \varepsilon_{n+k}. \end{aligned}$$

The result follows from this by an application of Lemma 4, with  $z_m = r_m$ ,  $\Lambda = \varepsilon$ ,  $N = (x_n - a)/h$  and  $Z=0$  (i.e.  $r_0 = r_1 = \dots = r_{k-1} = 0$ ).

It thus follows from Theorems 1-3 that the H-optimal multistep methods of the thesis continue to enjoy the approximation properties of the corresponding consistent and stable usual methods in addition to being optimal (or quadrature optimal) methods in the Hilbert space set up.

The numerical results of the previous chapters show amply clearly the enhanced accuracy advantage of H-optimal methods over the usual ones.

The only disadvantage of H-optimal methods seems to be the storage requirement for the variable coefficients of these methods. However, for the present day computers, this much amount of storage is not really a problem.



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## APPENDIX

### DISCUSSION AND SUGGESTIONS FOR FUTURE RESEARCH

As we have mentioned in the beginning, 'the present thesis may be regarded as a first exploratory study of Sard's approach to optimal multistep methods'. The findings by now may be summarised as follows:

(a) By definition, the methods have been derived for certain spaces of functions (namely,  $H^2(C_r)$  and  $L^2(\ddot{C}_r)$ ) as a whole. This entails an *a priori* assumption that we are dealing with equations whose solutions are from these spaces. (b) The formulae are characterized by their being interpolatory for certain local functions and their behavior (c) as  $r \rightarrow \infty$  and (d) as step size  $h \rightarrow 0$  have been determined. It is shown that (e) under the hypothesis of Picard's theorem the methods are convergent. The important point about the convergence here is that there is no restriction on the solutions (that it be a member of the space of the derivation of the method). (f) The coefficients of the methods, which are variable, however, are shown to differ from those of the parent usual methods by  $O(h)$ ,  $h \rightarrow 0$ . (g)  $O(h^{p+1})$  bounds on local truncation errors are established, for  $p$ -th order parent methods in both implicit and explicit cases. Also, (h) bounds for discretization & (i) round off errors have been obtained which as far as the order is concerned parallel those of the parent usual methods. (j)

The numerical experiments on two dozen problems, conducted on a fixed step size basis, has given encouraging results.

The present work is limited by obvious considerations, not the least amongst them being due to the mist that surrounds the beginnings of any new approach. For instance the analytical derivation, coupled with the  $O(h)$  closeness of the coefficients, strongly suggests an asymptotic expansion in powers of  $h$  which will not only result in clearing up questions related with various notions of stability and sharper asymptotic behavior of the numerical solutions, but will also facilitate a computation of the coefficients specially required in an adaptive implementation of the methods with stepsize control.

Several aspects of the problem which we could not study concern: (a) various notions of stability, (b) stiff and singular equations, (c) system of equations, (d) initial and boundary value problems for higher order equations, (e) special classes of differential equations, (f) any serious study of formulae interpolatory for any specific functions that have been studied earlier in other context e.g. by Gautschi [A8], Lambert [A12], Lanczos [A14], Cash [A3], Corrol [A5], Iserles [A11], and Neta and Ford [A15] etc. (Our motivation regarding this point came from the work of Chawla and Kaul [16-18], Kaul [30] and Finney and Price, Jr. [24] as mentioned in the first chapter.), (g) spaces other than  $H^2(C_r)$

and  $L^2(\hat{C}_r)$  and  $\langle h \rangle$  experiments with different values of  $r$  for problems for which solutions are expected to be with a graded smoothness.

We acknowledge that in order to take extra advantage of the accuracy that these optimal formulae deliver, it is critical that  $r$  be chosen with care. From an intuitive standpoint, as a general guideline,  $H^2(C_r)$  and  $L^2(\hat{C}_r)$  with a smaller  $r$  would be more appropriate when the actual solution is expected to be less smooth and a larger value of  $r$  for solutions with a higher smoothness.

This is also in agreement with the following table in which we give the ratio, for the Problems 3 and 4, of relative errors of optimal as compared with the usual methods in the case of explicit methods :

Table A1

Ratio of end point ( $x_N=1.2$ ) relative errors for problems 3 & 4

Table No.	-----Multistep Method (EXPLICIT)-----					
	M	M <sup>1</sup>	M <sup>2</sup>	M <sup>3</sup>	M <sup>4</sup>	M <sup>F</sup>
2.9	10.373	10.730	11.803	11.366	17.049	11.803
3.9	8.119	7.344	17.106	8.115	3.653	10.882
4.9	9.570	9.708	12.490	10.230	64.728	11.177
5.9	6.557	5.987	5.656	6.833	2.985	12.787

We note that the singularity in Problem 3 is nearer the circle  $C_r$  than it is for Problem 4, and the methods perform

relatively much better when the singularity is nearer. Moreover, in the quadrature optimal cases the gains are relatively higher as compared to the optimal cases.

The corresponding table in the implicit case is as follows:

Table A2

Ratio of end point ( $x_N=1.2$ ) relative errors for problems 3 & 4

Table No.	-----Multistep Method (IMPLICIT)-----						
	M	M <sup>1</sup>	M <sup>2</sup>	M <sup>3</sup>	M <sup>4</sup>	M <sup>5</sup>	M <sup>F</sup>
2.10	1.937	1.959	1.796	2.143	1.431	2.724	1.760
3.10	0.825	-0.586	1.139	-0.421	0.913	-0.144	8.716
4.10	3.632	4.059	1.780	7.263	1.162	4.292	2.270
5.10	0.145	-0.279	0.660	0.250	0.744	0.312	-7.263

In the above table, we observe that in the implicit case the performance of quadrature optimal methods (corresponding to Tables 2.10 and 4.10) in all cases is as stipulated. In the optimal cases (corresponding to Tables 3.10 and 5.10), however, there is no consistent pattern. This may be because for both the Problems 3 and 4 the errors are already quite small and are of both positive and negative signs.

In this connection, a theoretical determination of  $r$ , unfortunately involves a (hitherto unavailable) knowledge about the degree of approximation



$$E_r(y, \lambda) = \inf \{ \|y - g\|_S : g \in X_r, \|g\| \leq \lambda \},$$

where  $X_r = H^2(C_r)$  or  $L^2(\hat{C}_r)$ ,  $\|\cdot\|_r$  is the norm in  $X_r$  and  $\|\cdot\|_S$  is an appropriate norm for the solution space (e.g.,  $\|y\|_C + A \|y'\|_C$ ,  $\|\cdot\|_C$  denoting the sup norm). This is because a tighter bound for the local truncation error is given by

$$\|T_n(y)\| \leq \inf_{\lambda > 0} \{ E_r(y; \lambda) + \lambda \|T_n\|_r \}.$$

In view of the above, in a practical situation a determination of  $r$ , right now, lies in the domain of experimentation.

In the thesis we have mostly concentrated on theoretical aspects and there too on only those for which we had something definite to say. Thus, there remains a lot of work to be done both in theoretical as well as practical directions. Concerning stability, for instance, we have been involved only with the weaker version when the characteristic polynomial of  $a$ 's is stable (i. e. its roots are on or inside the unit circle and those of modulus 1 are simple). Even though for the mere convergence it is enough (as follows from Theorem 1 Chapter 6), for stronger versions and for avoiding other type of numerical instabilities one has to work with only those optimal methods which correspond to usual methods possessing the appropriate stability. Thus, for instance, in the quadrature optimal methods with  $s \neq 0$ , parasitic roots could ruin the relative stability of the solution, and therefore

should not be applied for problems where this is important.

The note at which we ended Chapter 6 is based on our numerical experience for a fixed step size only, when the coefficients have already been determined. The practical situation, indeed, is far from it. For, fixed stepsize numerical results say little about the overall potential of the formulae. To be of any practical use these formulae must be competitive in a variable-step, variable-order environment. This requires an efficient separate routine for a determination of the variable coefficients of the optimal methods. This extra work involves setting up the linear system of normal equations and solving it. (If at a step one chooses  $m$  non-zero  $a$ 's and  $n$   $b$ 's, it involves  $(m+1+n)n$  function (kernel and its derivative, etc.) evaluations and about  $n^3/3$  arithmetic operations at that step.) The use of one or more parallel processors for this purpose has also to be investigated.

In the thesis we have considered only the scalar case. However, in practice one comes across the vector case of systems of equations, in which, all the more, different components might possess different degrees of smoothness. In principle, the ideas of the thesis naturally extend to this case in a similar fashion (in about the same way as the proof of Picard's theorem generalizes from the scalar to the vector case). Here the inner product for the product space would be

$$(y, z) = \sum_i (y_i, z_i)_{H_i},$$

where  $H_i$  is a space of choice for the  $i$ -th component. Thus  $H_i$ 's could be  $H^2(C_r)$  or  $L^2(\hat{C}_r)$ , with the same or different  $r$ 's, or they might be some other spaces altogether. It may be noted here that if the  $a$ 's and  $H_i$ 's to each component are the same, the coefficients of the optimal formula coincide with those of the scalar case. However if the  $b$ 's are kept independent for each component the normal equations decouple with each other with respect to  $H_i$ 's. The earlier discussion regarding the choice of  $r$  applies *mutatis mutandis* to this case, making it clear that this product also needs a lot of future investigation.

A step size control for a predictor - corrector pair is made possible in our case by Lemma 6, Chapter 6. If the predictor - corrector usual formulae are respectively of  $p$ -th and  $(p+1)$ -th order, so are the related optimal formulae, by the lemma. Thus, following Cash [A3] and Shampine and Gordon [A21], we may use the standard strategy :

With  $y(x_{n+1})$  as the exact solution,  $\bar{y}_{n+1}$  the predicted value and  $y_{n+1}$  the corrected value at  $x_{n+1}$ ,

$$y(x_{n+1}) = \bar{y}_{n+1} + O(h^{p+1}),$$

and 
$$y(x_{n+1}) = y_{n+1} + O(h^{p+2}).$$

If  $O(h^{p+2})$  terms are neglected,  $TE = y_{n+1} - \bar{y}_{n+1}$  is an estimate for the local truncation error for  $\bar{y}_{n+1}$  and it is this error which we will control. The scheme is based on local

extrapolation, that is our error estimate is for the predicted solution  $\bar{y}_{n+1}$ , while it is the asymptotically more accurate solution  $y_{n+1}$  which is actually carried forward. This procedure, where the step control algorithm is based on an estimate of the local error in the predicted, rather than the corrected solution, is a common one. With TE as before in the scalar case (and putting  $TE = \| y_{n+1} - \bar{y}_{n+1} \|_{\infty}$  , in a vector case) and denoting the local accuracy required by  $\epsilon$ , the way in which the step size is controlled, when using p-th order formula, is as follows :

- (i) If  $TE > \epsilon$ , halve h and recompute the solution at  $x_{n+1}$ ;
- (ii) If  $\epsilon \geq TE \geq \epsilon/2^{p+1}$ , accept the solution and keep h fixed;
- (iii) If  $TE < \epsilon/2^{p+1}$ , accept the solution and double h.

It may be remarked here that we do not know presently whether our optimal formulae possess the usual type of asymptotic error estimates, and consequently a step size control with respect to the corrector is faced with difficulties.

Finally a list of some additional and recent references on multistep methods, which could not find place in the main body of the thesis, follows:

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